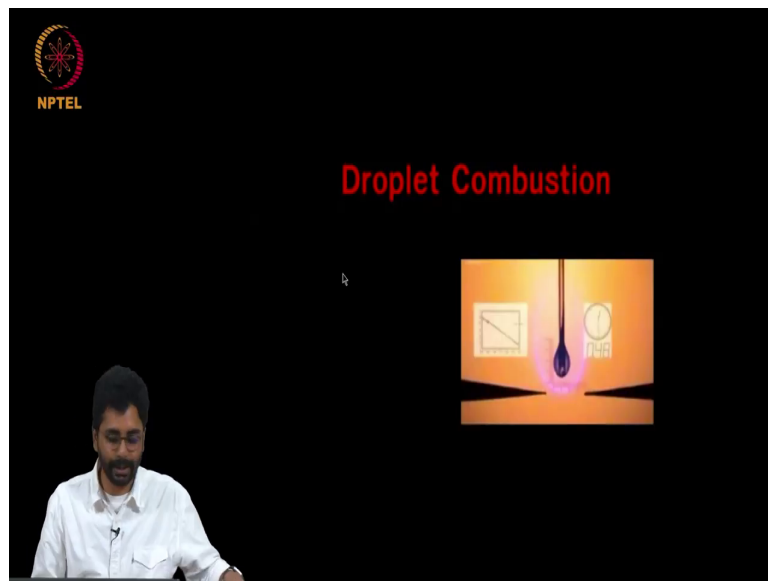


Fundamentals of Combustion for Propulsion
Prof. S Varunkumar
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture - 06
Demonstration of NASA-CEA

(Refer Slide Time 00:16)



Welcome back. We starting a little early than I mentioned. So, what I thought was I used the droplet a picture from the droplet combustion video to bring out the idea of equilibrium versus rate controlled processes and combustion, maybe I will start I thought I will start by showing you a video of droplet combustion.

(Refer Slide Time 00:45)



This is an important process that occurs in burners, reciprocating engines and gas turbines. It is captured by burning droplets on a quartz fiber at normal gravity. You will see the following fuel droplets being burnt.

1. Ethanol
2. Gasoline
3. Kerosene
4. Diesel

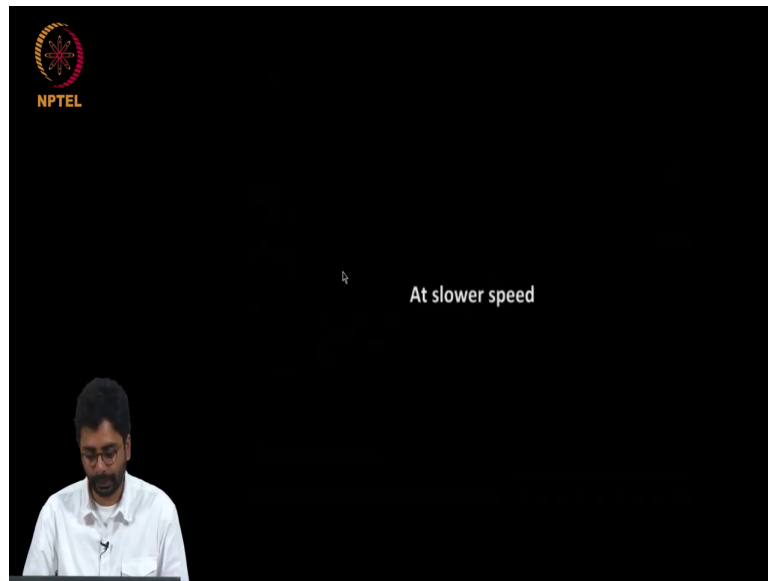
Ignition: Electric spark

Red dot shows the path of equivalent droplet diameter with time

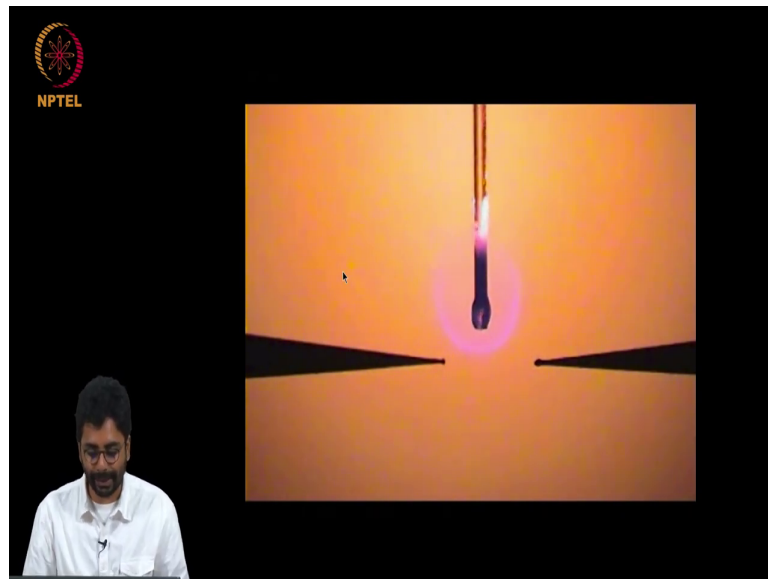


This is the video from which the picture was taken.

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(Refer Slide Time 00:52)



There is also audio, good. I think you can clearly see the flame in this case and along with the droplet.

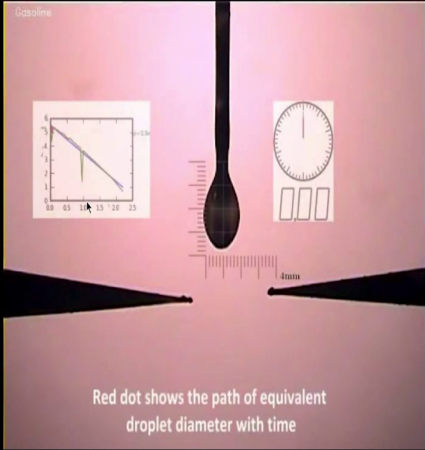
(Refer Slide Time 01:05)



(Refer Slide Time 01:06)

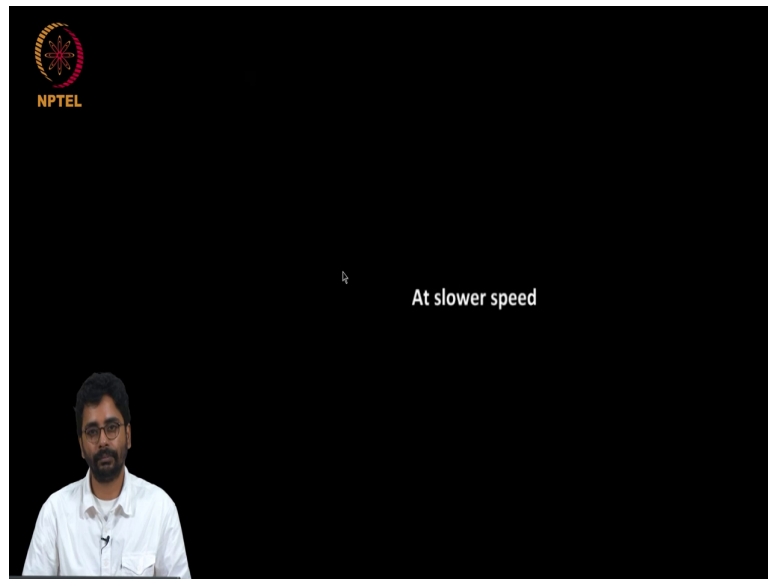


NPTEL

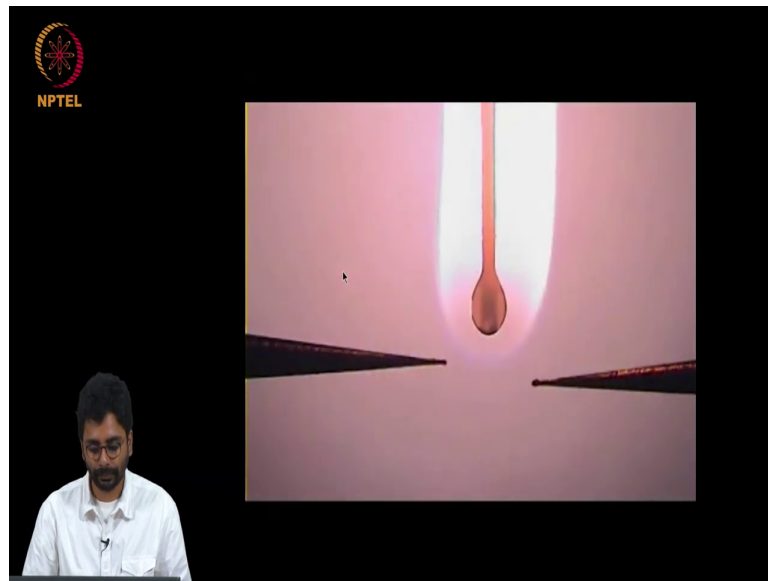


Red dot shows the path of equivalent droplet diameter with time

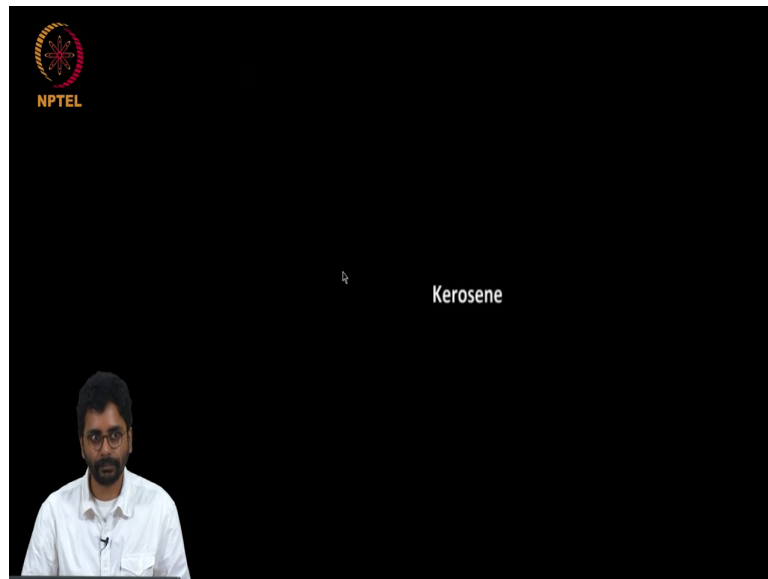
(Refer Slide Time 01:10)



(Refer Slide Time 01:13)



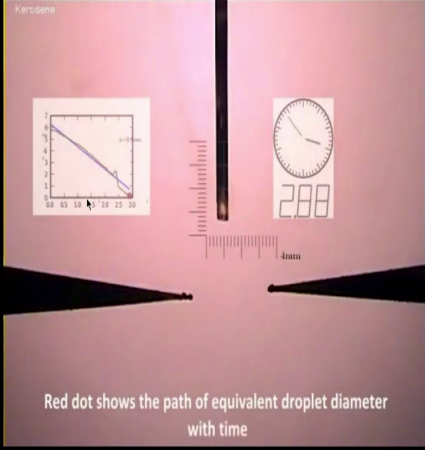
(Refer Slide Time 01:22)



(Refer Slide Time 01:24)

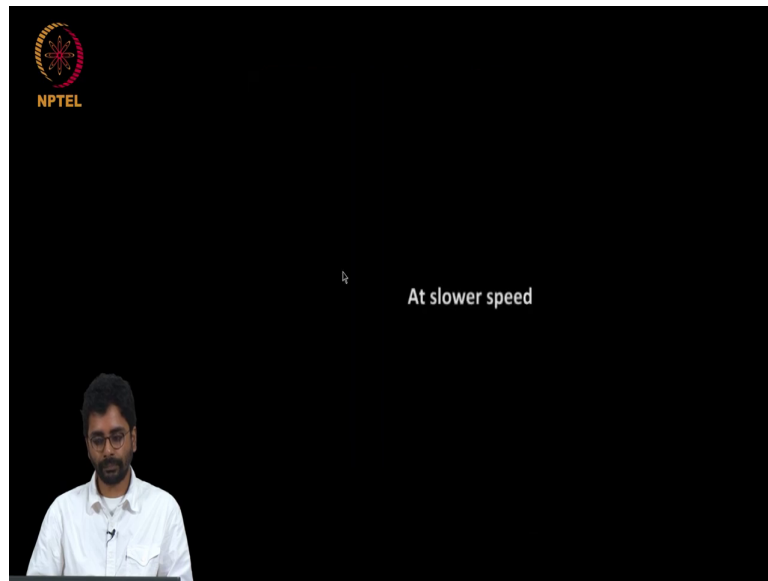


NPTEL

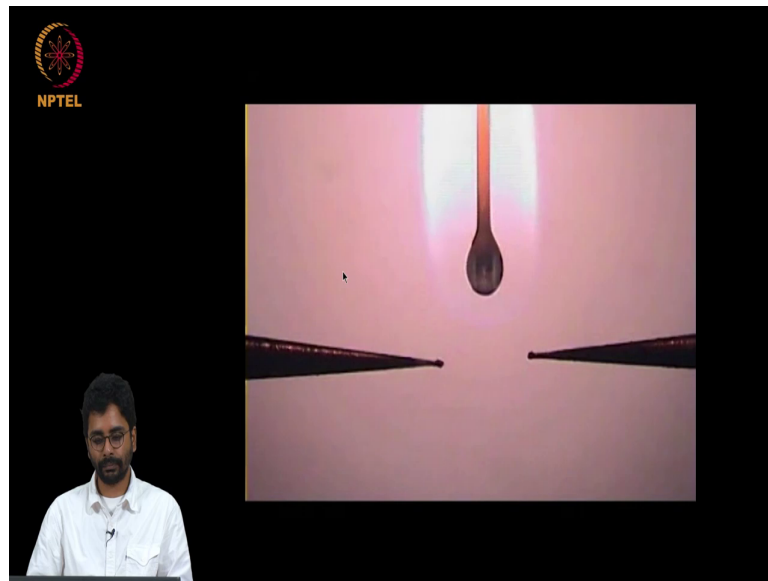


Red dot shows the path of equivalent droplet diameter with time

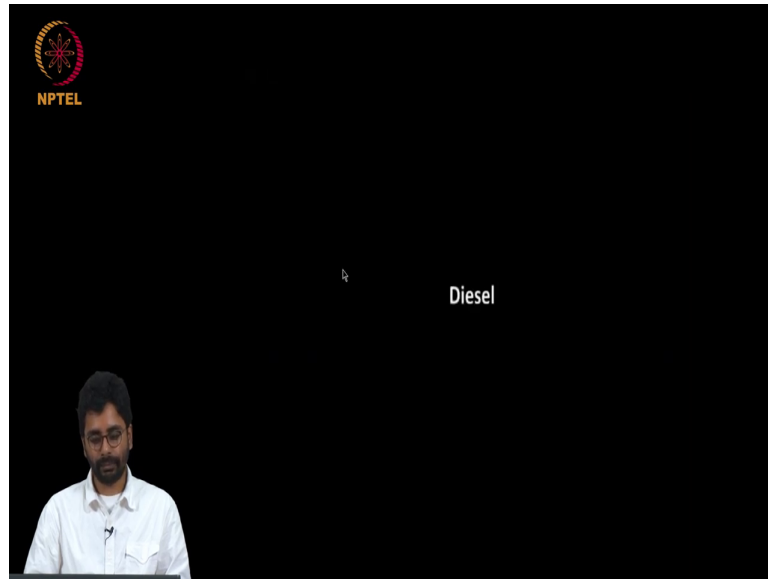
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(Refer Slide Time 01:32)



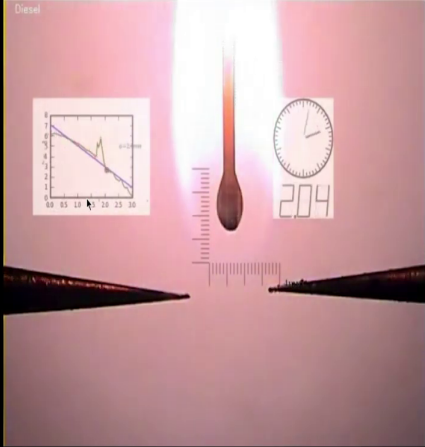
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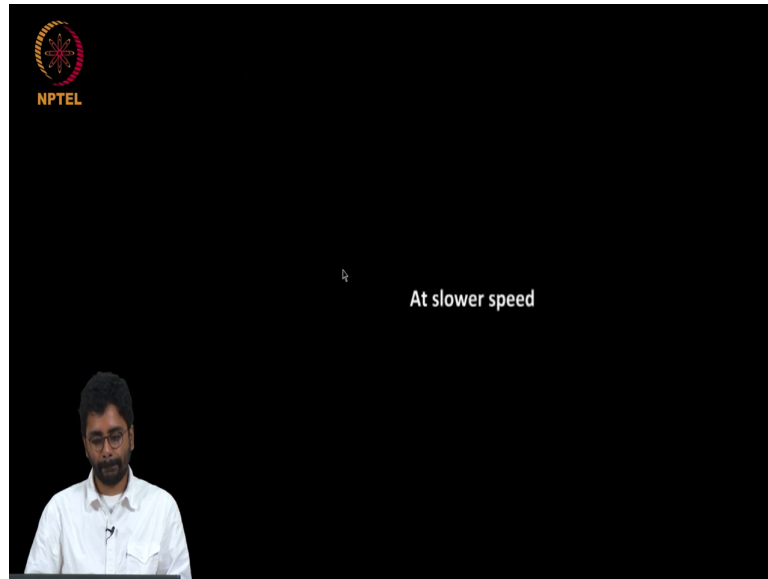


NPTEL

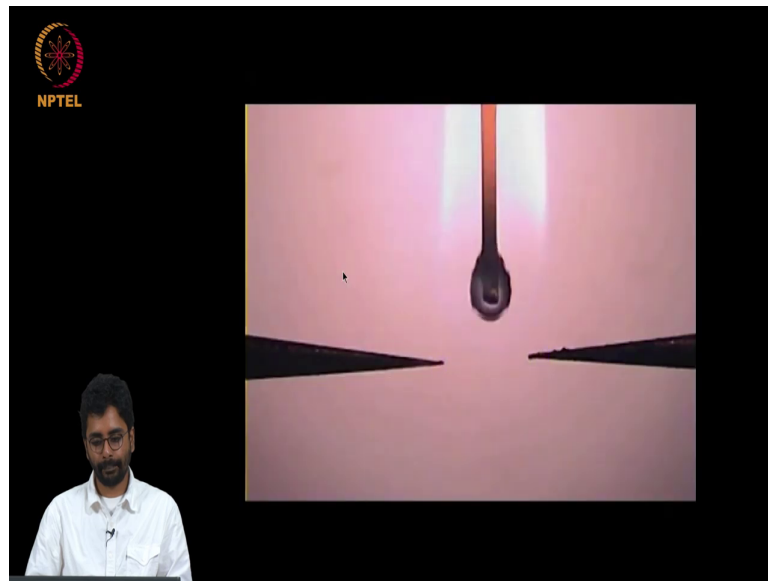


The composite image displays four elements: a graph on the left, a thermometer in the center, a clock on the right, and a digital display showing '204' at the bottom right. The graph has a y-axis from 0 to 8 and an x-axis from 0.0 to 3.0. The thermometer shows a red liquid level. The clock shows a time around 1:50. The digital display shows '204'.

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Composite picture of fuel droplet combustion

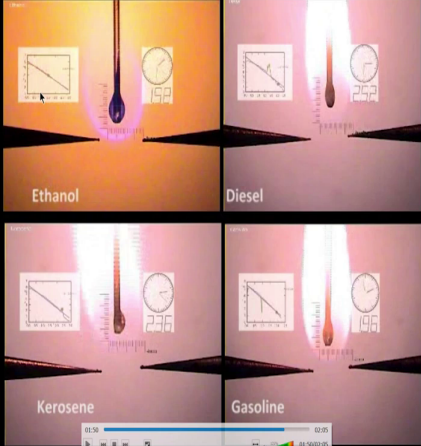
Note the transparency of ethanol flame compared to others



(Refer Slide Time 02:07)



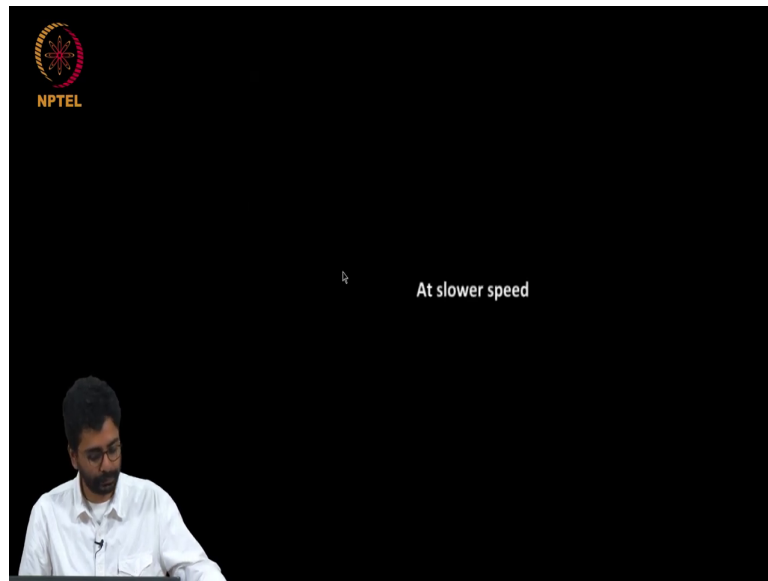
NPTEL



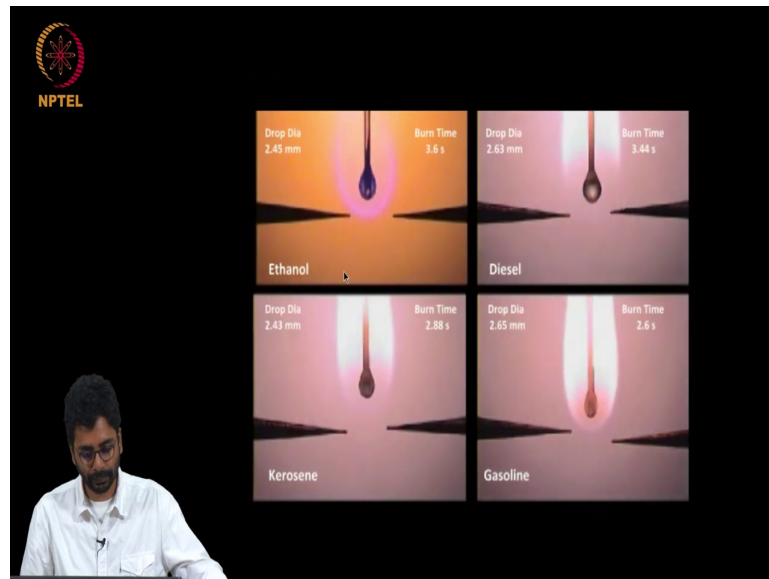
Substance	Temperature (°C)
Ethanol	152
Diesel	276
Kerosene	276
Gasoline	196

01:50 02:05

(Refer Slide Time 02:10)



(Refer Slide Time 02:12)



This so I think this is a good picture to show, at just a couple of things I want you to notice this is the droplet and the flame and the ignitor. And what is shown on the side plot is on the x axis there is time, and on the y-axis there is a diameter squared, the diameter sort of measured from the video processing of image processing of the video.

What I want to emphasize is that the by the droplet time is dependent on the square of the diameter, so that is a D -squared law as it is called. This is one example of a combustion process where chemistry has no role.

So, the time goes is diameter squared it simply depends on the transport processes occurring at the surface of the droplet, and the heat flux that the surface receives is dependent on the location of the flame which again is controlled by mixing and not by reaction rates ok. Of course, there are lot of other complex things that happen for example, sometimes the droplet

boils and then show some erratic movement and that is what you see a fluctuations in d^2 , but the overall linearity of d^2 versus t is followed.

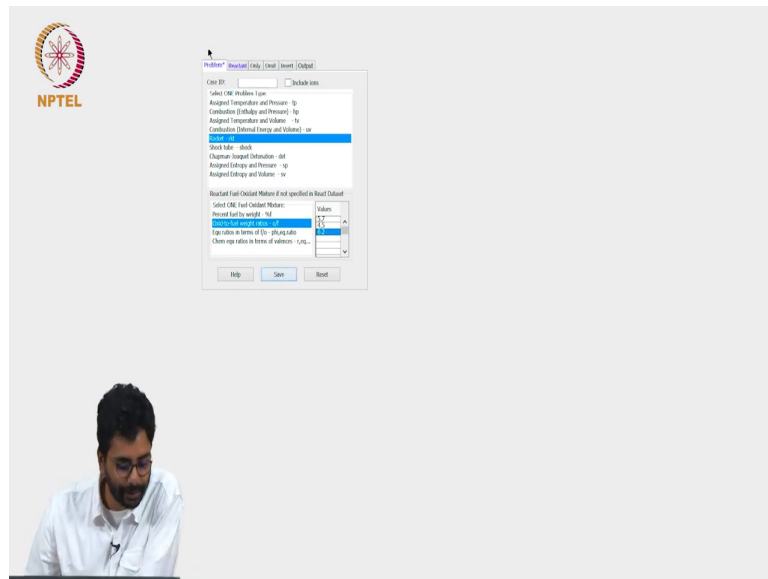
The other thing I want to emphasize is that some flames or only ethanol flame is non-luminous and it does not have a yellow color ok. All the other fuels have a luminous flame and yellowish flame like a candle flame. And all these are kerosene, gasoline and diesel are mixtures of hydrocarbons with carbon number of at least 6 or 7 ok. So, these kind of and ethanol of course is a pure substance and has only a two carbon atoms ok.

So, these other fuels have a tendency to coke or form soot that is one more thing I wanted to emphasize. And therefore, the kind of modeling approach that is required is dependent on what phenomena you are interested in capturing. If you want to get this you know explain only the d^2 versus t and get an estimate of the slope of the line, and there is a certain kind of approach that will work.

But if you are interested in kerosene droplets being injected into a complex rocket combustion environment where you are interested in understanding whether that system you go in to instability or not, you require a certain kind of approach. Or if you are interested in emissions from let us say a reciprocating engine using one of these fuels, then you need a then you have no option, but to actually include some level of description of chemistry in your calculations to predict emissions ok, because the emission formation is a kinetically controlled process ok.

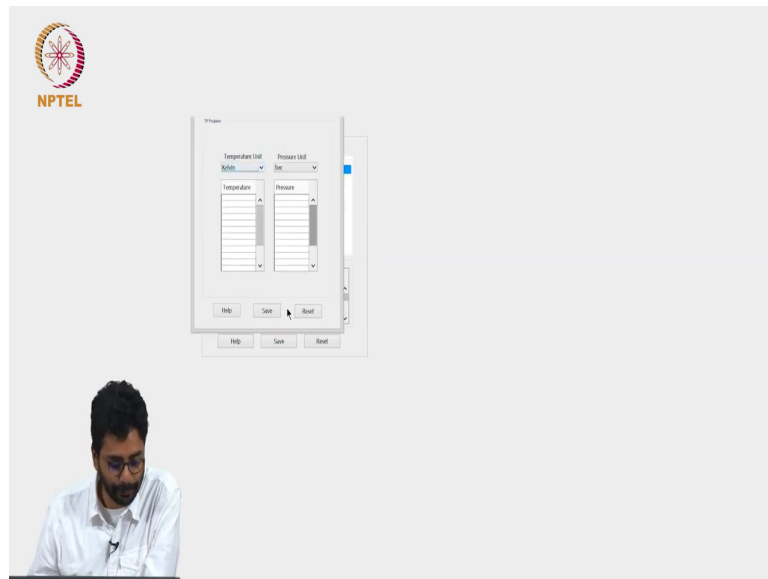
So, perhaps a hierarchy of approach is what is suggested when taking a modeling approach to understanding systems. I just thought I will show this example and because we discussed this in the morning.

(Refer Slide Time: 05:02)



With that I would like to move on to the demonstration of NASA CEA. CEA stands for Chemical Equilibrium and Analysis. I am sure participants from ISRO and DRDO are quite familiar with this tool, and they must be using it on a daily basis. But for the benefit of the others I thought we will look at a few example cases ok.

(Refer Slide Time: 06:32)



So, this is the when you open the software, this is the first page that you see there are different problems that are listed here, different types of problems that are listed here. You can calculate equilibrium states under a variety of constraints. So, you can calculate equilibrium states that the temperature and pressure fixed that is the first option. The second one is with the enthalpy and pressure fixed that is the h and p problem.

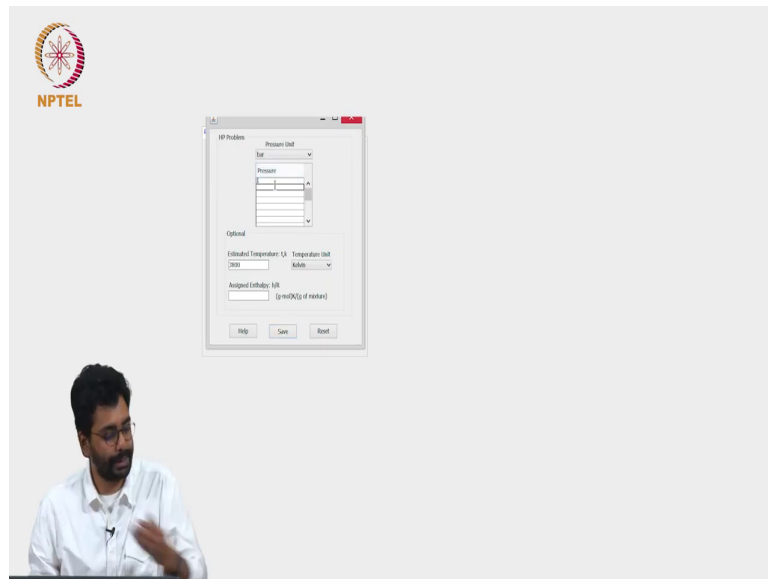
And the third one is the temperature and the volume fixed, the fourth one is internal energy and volume fixed ok. We saw in the morning that the first law of thermodynamics applied to applied to a mixture of fuel and oxidizer at a certain initial temperature and pressure when you are interested in calculating adiabatic flame temperature falls either in one of these two categories, it could be a constant pressure or constant volume.

For example, if you are analyzing a rocket combustion chamber, you will assume that the pressure is constant and if you are analyzing spark ignited internal combustion engine, then you will assume that the combustion is happening under constant volume conditions. And under constant pressure and adiabatic conditions the first law says that the enthalpy should be fixed.

We saw in the morning that the enthalpy of the reactants must be equal to enthalpy of the products. And under constant volume conditions, it will become volume is fixed and the internal energy is fixed ok. This is the constraint that comes from the first law. The second law constraint is that in the h, p problem. In the h, p problem in the h, p problem that the Gibbs free energy must be minimized, and then the u, v problem the (Refer Time: 08:21) free energy must be minimized.

So, the h, p constraint comes from the first law; the other constraint comes from the combination of first law and second law. In fact, the software calculates the equilibrium states by minimizing the Gibbs free energy function using Lagrange multipliers ok. Instead of setting I think I will set up a problem let us look at the example case that we discussed in the morning.

(Refer Slide Time: 08:54)



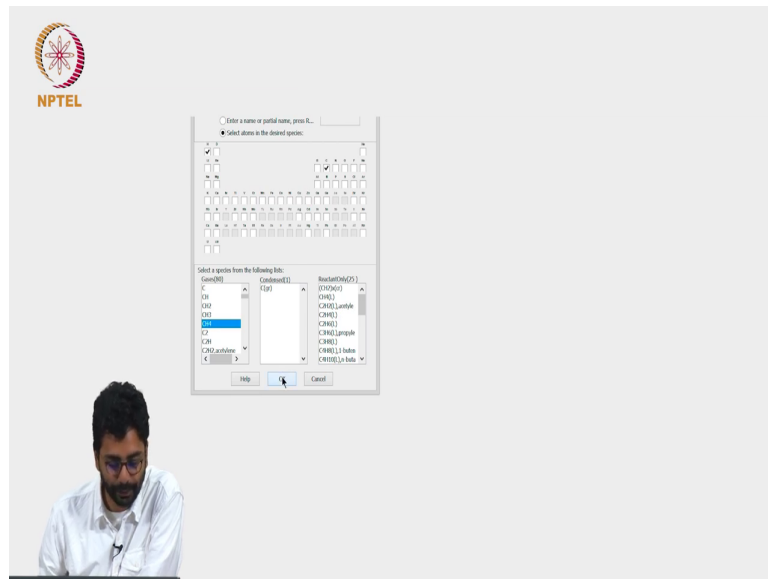
Determining the adiabatic flame temperature of let us say methane and air mixtures at different stoichiometric values at [noise let us say three different pressures 1 bar, 5 bar and 10 bar ok. So, I am assigning three different pressures, calculation will be done at three pressure values 1 bar, 5 bar and 10 bar ok. So, this is what you first you pick which problem you want to solve, then you fix the pressure because you have to specify a pressure.

(Refer Slide Time: 09:26)

The NPTEL logo is located in the top left corner. It consists of a circular emblem with a stylized sun or flower design in the center, surrounded by a ring of red and white segments. Below the emblem, the letters "NPTEL" are written in a bold, orange, sans-serif font.

Then we move on to the second tab where you can specify the reactants.

(Refer Slide Time: 09:31)



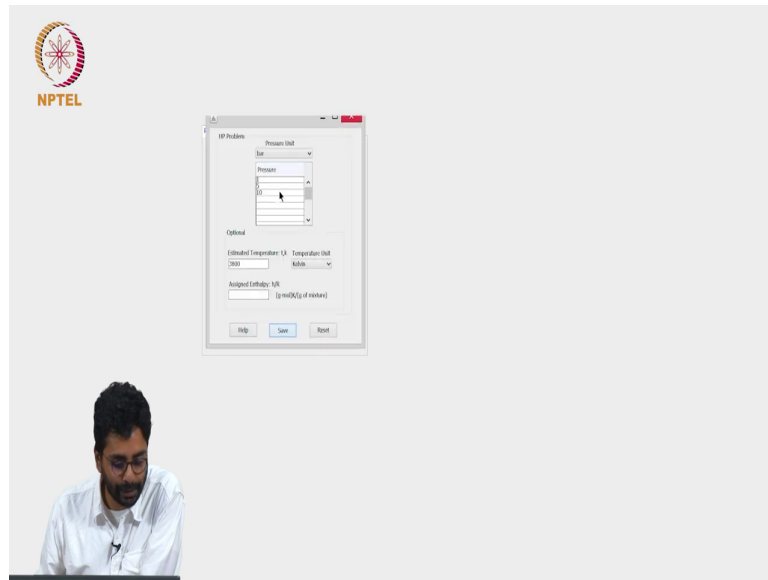
Well, there is already hydrogen and air, but let us try methane CH_4 of course, you will have different version CH_4 naturally occurring from gaseous, but there is also liquid methane which somebody may want to use for a rocket calculation for example, ok.

Well, let us you have two options either to specify the relative number of moles right here ok, but we will not do that we will just specify the initial temperature 300 Kelvin's and 300 Kelvin's ok. The stoichiometric can be specified separately here either as a equivalence ratio or oxidation to fuel weight ratio or percentage fuel all are equivalent, but only that the numbers must be consistent. So, let us try a equivalence ratio in terms of ϕ I will pick one value for lean, stoichiometry and rich ok.

I will do a quick recap. We first pick the problem we have pick the enthalpy pressure problem. You can assume let us say we are interested in determining adiabatic flame temperature for a

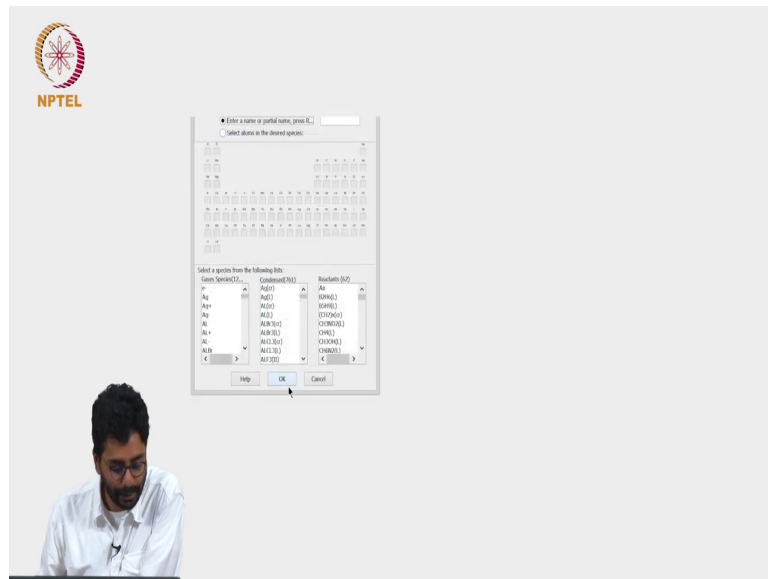
combustion device, it is going to operate at constant pressure with let us say atmospheric pressure with methane and air as fuel. Let us say the open flame that we discussed in the morning.

(Refer Slide Time: 10:56)



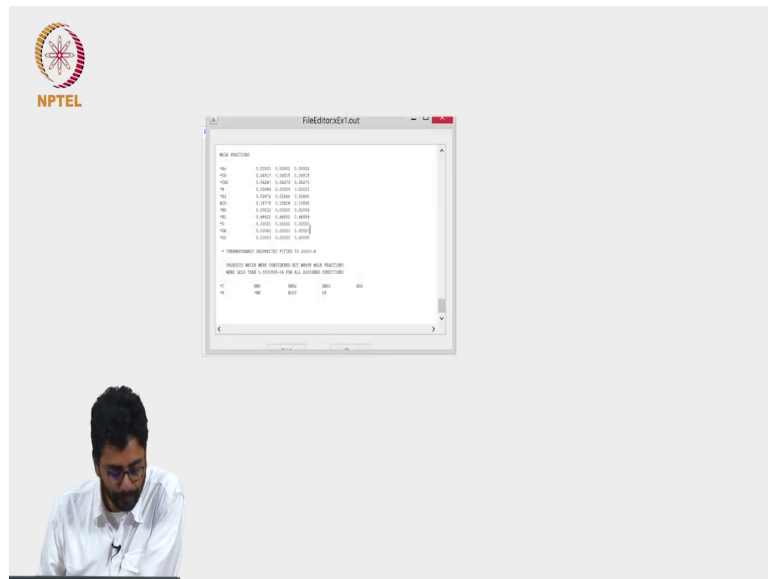
Then we assign pressure values 1, 5, and 10 bar. Just to look at the effect of pressure.

(Refer Slide Time: 11:03)

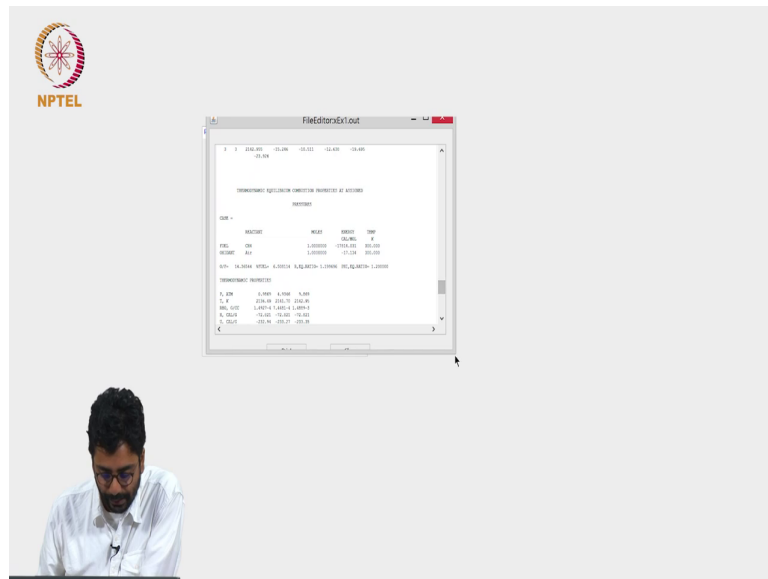


And then we pick the reactants, the fuel is methane the oxidizer is air both are at 300 Kelvin's of course, I can I have specified I can specify the relative amounts here, so that the certain stoichiometry is maintained, but I can also specify the values here which is what I have done. Let us run the calculation and see what we get ok.

(Refer Slide Time: 11:22)



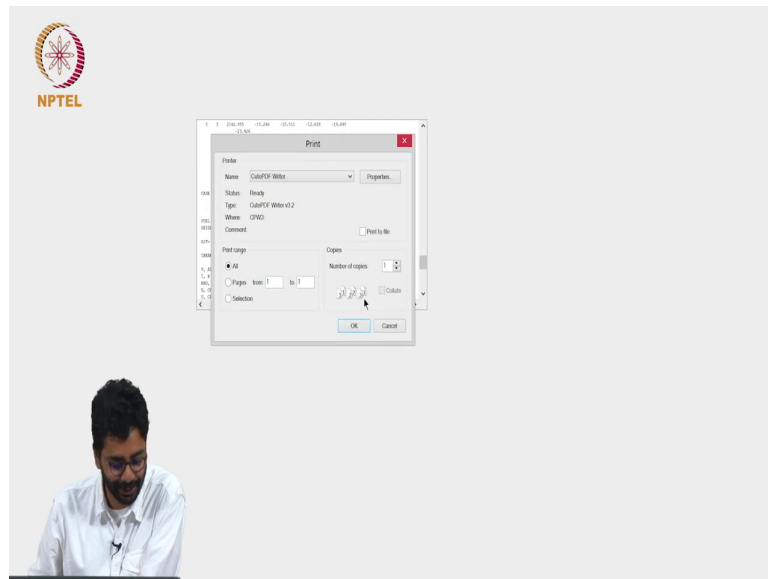
(Refer Slide Time: 11:26)



So, these are the results. The fuel is a methane oxidant is air. For a phi of a points the for a phi of 1.2 which is fuel rich, the oxidizer to fuel ratio is 14.36 which I think is a you do not know how this can be made bigger than this.

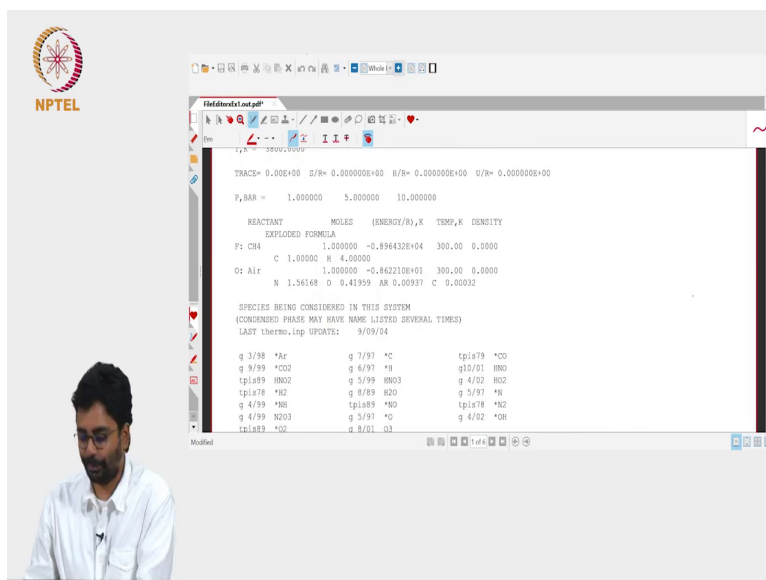
Student: (Refer Time: 11:56).

(Refer Slide Time: 11:57)



All right, thank you.

(Refer Slide Time: 12:09)

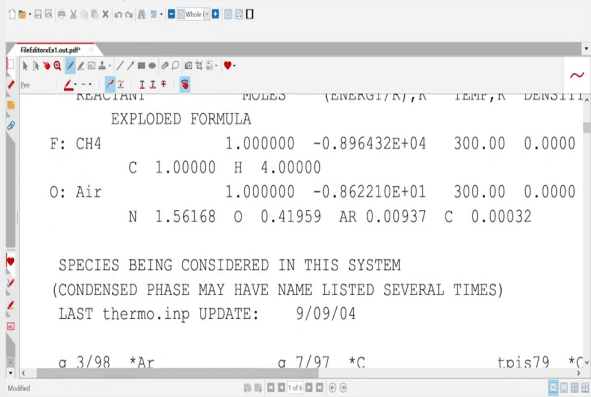


Sorry, I think I am, nice.

Student: (Refer Time: 12:13).

Good enough, (Refer Time: 12:16) little further also I guess ok.

(Refer Slide Time: 12:19)



The screenshot shows a software window titled "thermo.inp.pdf" with a menu bar (File, Edit, View, Tools, Windows, Help) and a toolbar. The main content area displays the following text:

EXPLODED FORMULA

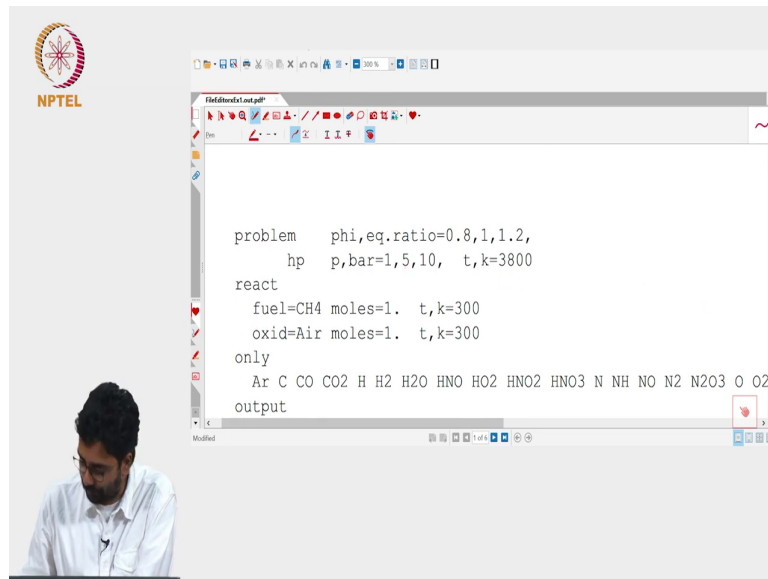
REACTANT	MOLES	(ENERGY/KJ,K	TEMP,K	DENSITY
F: CH4	1.000000	-0.896432E+04	300.00	0.0000
C	1.000000	H 4.000000		
O: Air	1.000000	-0.862210E+01	300.00	0.0000
N	1.56168	O 0.41959	AR 0.00937	C 0.00032

SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)
LAST thermo.inp UPDATE: 9/09/04

At the bottom, there is a status bar with the text: "α 3/98 *Ar α 7/97 *C tois79 *C" and a "Modified" label.

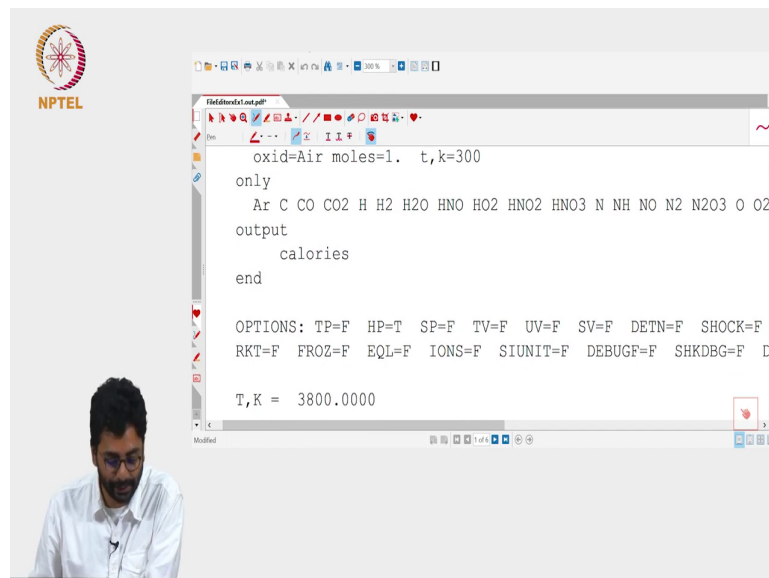
It is much better.

(Refer Slide Time: 12:34)



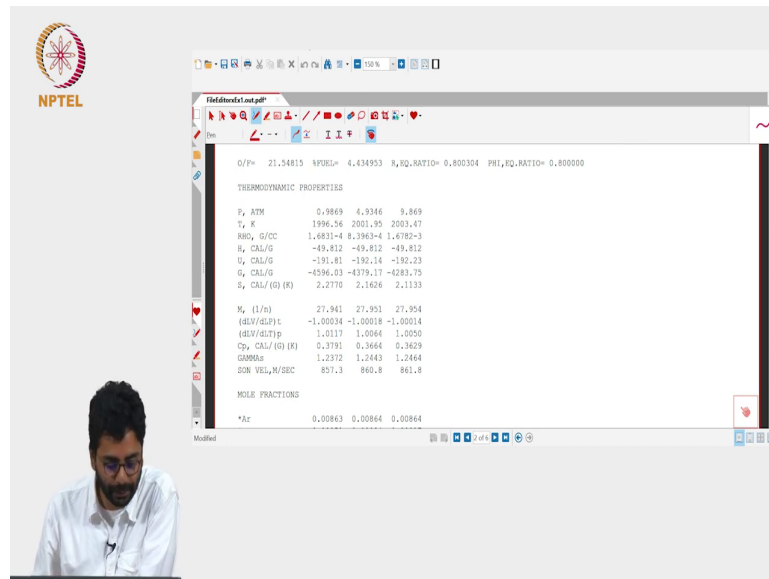
So, the fuel is, so we are specified the three equivalence ratios 0.8, 1 and 1.2, three pressure values 1, 5 and 10 bar do not worry about the temperature that is only a estimate of the temperature that is provided for an initial guess.

(Refer Slide Time: 12:45)



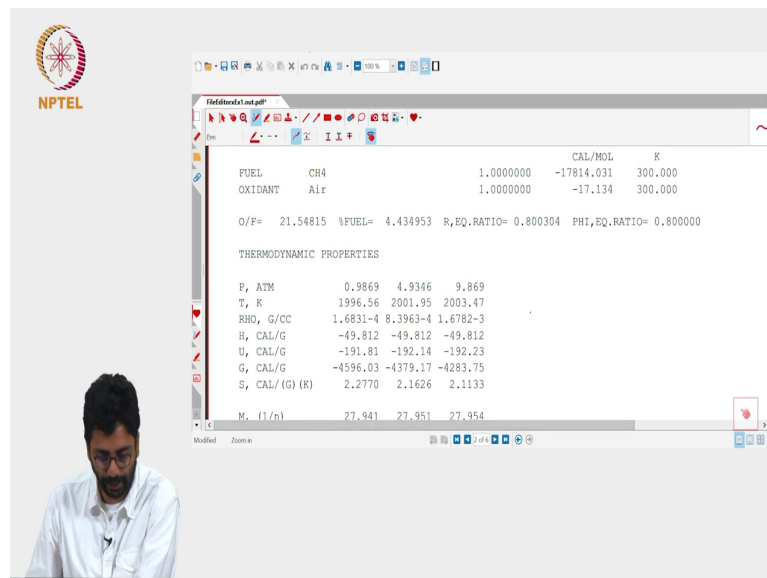
The reactants are methane and the oxidizer is air, these are the species that are considered in the equilibrium calculation. I have not gone into the details actually you need to now pick a set of reactions which are linearly independent, and then make and linearly independent, so that all the species that you have identified can be mole fraction of all those species can be calculated, then you apply the constraint of enthalpy being constant term ok, and minimize the Gibbs free energy after that.

(Refer Slide Time: 13:40)



Let us go to the results now. This is the case with the phi equals point h phi equals 1 we saw that the air to fuel ratio must be 17.16 in the example that I showed you in the morning. So, this seems consistent this is 21.4 because it is lean ok. And the calculation has run for three values of pressure, I gave 1 bar, 5 bar and 10 bar the now I will do that. Calculation has this is might easy to navigate 1 second ok.

(Refer Slide Time: 14:25)



The screenshot displays a software window titled "firedhsrds1.out.pdf" showing thermodynamic properties for a mixture of CH₄ (FUEL) and Air (OXIDANT). The properties are listed in a table with columns for units and values. The table is as follows:

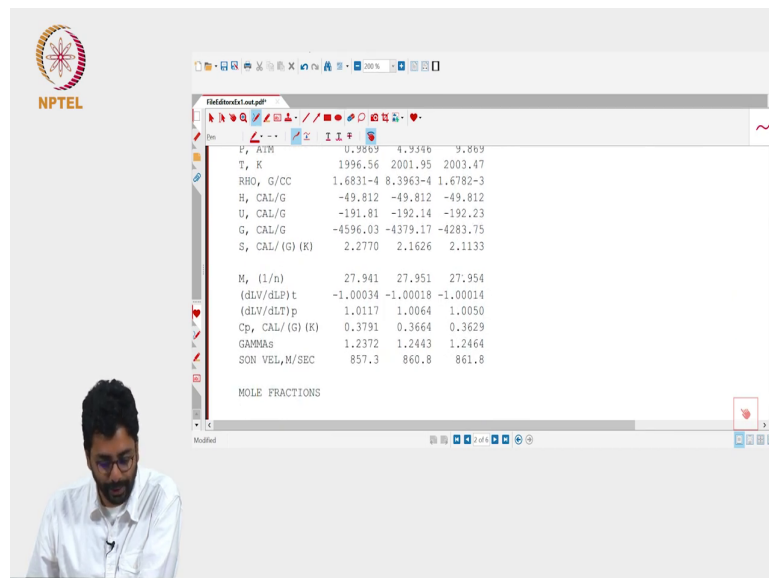
			CAL/MOL	K
FUEL	CH ₄	1.0000000	-17814.031	300.000
OXIDANT	Air	1.0000000	-17.134	300.000
O/F=	21.54815	%FUEL=	4.434953	R,EQ.RATIO= 0.800304
				PHI,EQ.RATIO= 0.800000
THERMODYNAMIC PROPERTIES				
P, ATM	0.9869	4.9346	9.869	
T, K	1996.56	2001.95	2003.47	
RHO, G/CC	1.6831-4	8.3963-4	1.6782-3	
H, CAL/G	-49.812	-49.812	-49.812	
U, CAL/G	-191.81	-192.14	-192.23	
G, CAL/G	-4596.03	-4379.17	-4283.75	
S, CAL/(G) (K)	2.2770	2.1626	2.1133	
M, (l/n)	27.941	27.951	27.954	

The video feed shows a man in a white shirt looking at the screen.

So, is it now? So these numbers are expressed in atmospheres, therefore it is a factor of 1.0, and 3 to 5 smaller than numbers and bar ok. So, that is why it is this number that is slightly lower than 1, slightly lower than 4 and so on.

So, let us look at the temperature values at 1 atmosphere the temperature at an equivalence ratio of 0.8 is about 1997 Kelvin's this is something that I mentioned as the pressure increases at the same equivalence ratio the same temperature increases a little bit because the extent of decomposition is lower, but the effect is not so significant once you go to very high values of pressure.

(Refer Slide Time: 15:15)



P, ATM	0.9869	4.9346	9.869
T, K	1996.56	2001.95	2003.47
RHO, G/CC	1.6831-4	8.3963-4	1.6782-3
H, CAL/G	-49.812	-49.812	-49.812
U, CAL/G	-191.81	-192.14	-192.23
G, CAL/G	-4596.03	-4379.17	-4283.75
S, CAL/(G) (K)	2.2770	2.1626	2.1133
M, (l/n)	27.941	27.951	27.954
(dLV/dLP)t	-1.00034	-1.00018	-1.00014
(dLV/dLT)p	1.0117	1.0064	1.0050
Cp, CAL/(G) (K)	0.3791	0.3664	0.3629
GAMMAS	1.2372	1.2443	1.2464
SON VEL, M/SEC	857.3	860.8	861.8
MOLE FRACTIONS			

So, I go from 1 bar to 5 bar, there is some change and then the change the delta keeps going down as you go to higher and higher pressures. This is one thing. There is also the molecular weight of the combustion products that are available which we will see will be useful for calculating or which is required for calculating the characteristic velocity in a rocket environment.

(Refer Slide Time: 15:25)

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File000001.txt.pdf

	0.3791	0.3664	0.3629
Cp, CAL/(G) (K)	0.3791	0.3664	0.3629
GAMMAS	1.2372	1.2443	1.2464
SON VEL, M/SEC	857.3	860.8	861.8

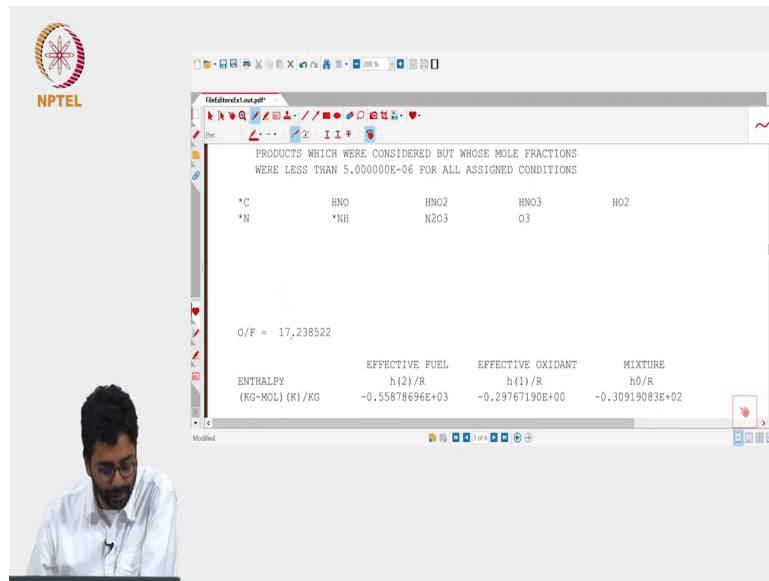
MOLE FRACTIONS

*Ar	0.00863	0.00864	0.00864
*CO	0.00051	0.00024	0.00017
*CO2	0.07702	0.07732	0.07740
*H	0.00002	0.00001	0.00000
*H2	0.00022	0.00010	0.00007
H2O	0.15333	0.15381	0.15395
*NO	0.00304	0.00308	0.00310

This is the product composition or the mole fractions of the product composition. Well, the point that I made that the dissociation of CO_2 is decreases with increase in pressure. So, you have more CO_2 at higher pressures, and far less CO at higher pressures at 10 bar compared to 1 bar. Similarly, for H also which anyway was very small at 1 bar, but it seems to be absent there is no H radical that is there at higher pressures ok.

So, dissociation is limited. Well, there is also some NO, but remember that these are equilibrium NO values. N₂ formation reactions are generally slow. So, this is how much NO you will have if you allow for very long time ok, but in the real system it is important to actually you know take into account the residence time for NO formation because the reactions are not as fast as the oxidation reactions. So, these are probably the upper limit can be considered as the upper limit of the NO that will form in these systems.

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PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

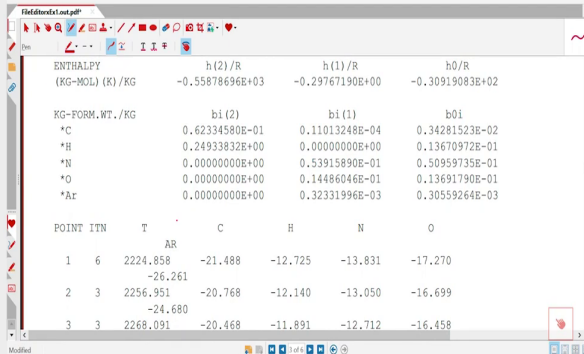
*C	HNO	HNO2	HNO3	HO2
*N	*NH	N2O3	O3	

O/F = 17.238522

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	h(2)/R	h(1)/R	h(0)/R
(KG-MOL) (K) /KG			
	-0.55878696E+03	-0.29767190E+00	-0.30919083E+02

And let us see this is the phi equals 1, phi equals 1 the O by F must be around 17.2 which is the case here.

(Refer Slide Time: 16:54)

ENTHALPY

(KG-MOL) (K) / KG	h(2) / R	h(1) / R	b0 / R
	-0.55878696E+03	-0.29767190E+00	-0.30919083E+02

KG-FORM. WT. / KG

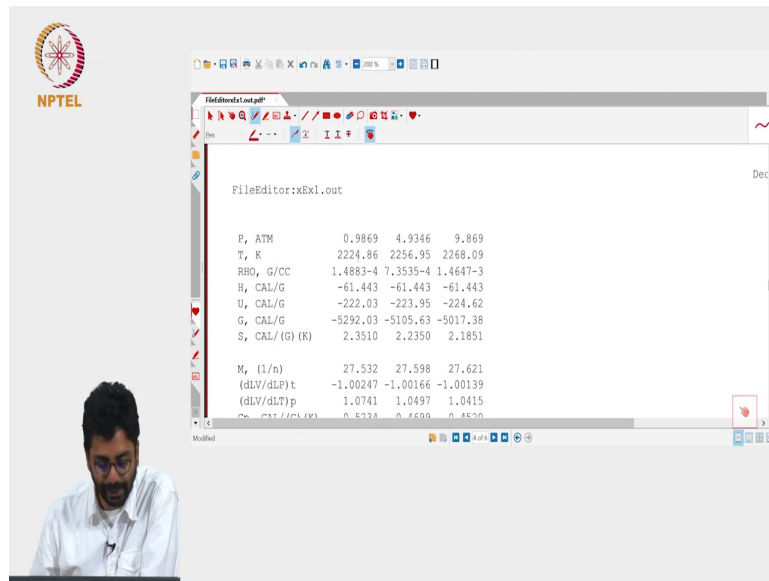
	bi (2)	bi (1)	b0i
*C	0.62334580E-01	0.11013248E-04	0.34281523E-02
*H	0.24933832E+00	0.00000000E+00	0.13670972E-01
*N	0.00000000E+00	0.53915890E-01	0.50959735E-01
*O	0.00000000E+00	0.14486046E-01	0.13691790E-01
*Ar	0.00000000E+00	0.32331996E-03	0.30559264E-03

POINT ITN T AR C H N O

1	6	2224.858	-21.488	-12.725	-13.831	-17.270
		-26.261				
2	3	2256.951	-20.768	-12.140	-13.050	-16.699
		-24.680				
3	3	2268.091	-20.468	-11.891	-12.712	-16.458

When I calculated, I did not take into account the traces of carbon dioxide and argon present in the air that is why I got 17.16, here those things are taken care of so that is why with 17.23, it is a small difference.

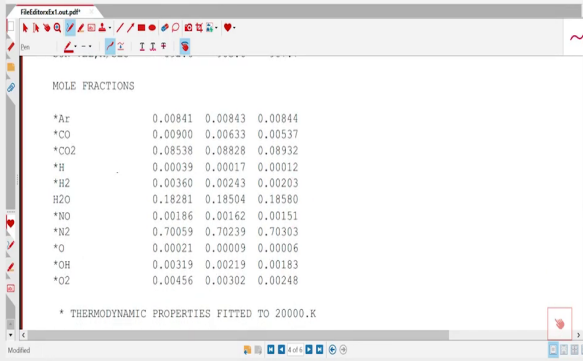
(Refer Slide Time: 17:16)



Property	Value 1	Value 2	Value 3
P, ATM	0.9869	4.9346	9.869
T, K	2224.86	2256.95	2268.09
RHD, G/CC	1.4883-4	7.3535-4	1.4647-3
H, CAL/G	-61.443	-61.443	-61.443
U, CAL/G	-222.03	-223.95	-224.62
G, CAL/G	-5292.03	-5105.63	-5017.38
S, CAL/(G) (K)	2.3510	2.2350	2.1851
M, (l/n)	27.532	27.598	27.621
(dLV/dLP)t	-1.00247	-1.00166	-1.00139
(dLV/dLT)p	1.0741	1.0497	1.0415
Sp, CAL/(G) (K)	0.5028	0.4500	0.4500

So, we expect that a ϕ equals 1 that the flame temperatures are higher than at ϕ equals 0.8, and which is the case we have gone from 1997 Kelvin's to about 2200, and as expected the temperature of the flame temperature also increases with increase in pressure ok.

(Refer Slide Time: 17:31)



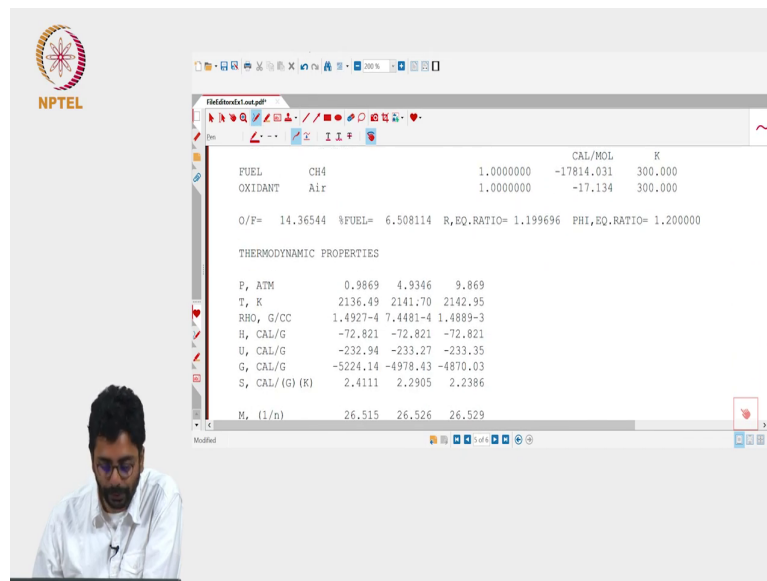
The screenshot shows a software window titled "THERMODYNAMIC PROPERTIES FITTED TO 20000.K". The window displays a table of mole fractions for various chemical species. The species are listed on the left, and their mole fractions are shown in three columns on the right. The species include Ar, CO, CO2, H, H2, H2O, NO, N2, O, OH, and O2. The mole fractions are numerical values ranging from 0.00000 to 0.18580. The window also includes a toolbar with various icons and a status bar at the bottom.

MOLE FRACTIONS			
*Ar	0.00841	0.00843	0.00844
*CO	0.00900	0.00633	0.00537
*CO2	0.08538	0.08828	0.08932
*H	0.00039	0.00017	0.00012
*H2	0.00360	0.00243	0.00203
H2O	0.18281	0.18504	0.18580
*NO	0.00186	0.00162	0.00151
*N2	0.70059	0.70239	0.70303
*O	0.00021	0.00009	0.00006
*OH	0.00319	0.00219	0.00183
*O2	0.00456	0.00302	0.00248

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

There are there is some Knox, there is also some oxygen. I just want to look at the rich condition and of course, the temperatures will be smaller as we expect.

(Refer Slide Time: 17:52)



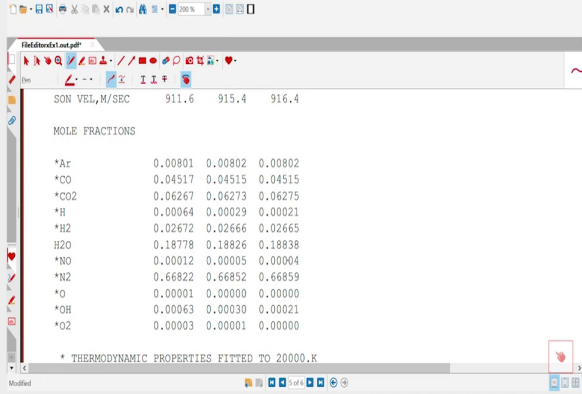
The screenshot displays a software window titled "firedhsrct1.txt.pdf" showing thermodynamic properties for a mixture of CH₄ (FUEL) and Air (OXIDANT). The properties are listed in a table with columns for the property name, units, and values for three different states.

		ATM	2141.70	2142.95
FUEL	CH ₄	1.0000000	-17814.031	300.000
OXIDANT	Air	1.0000000	-17.134	300.000
O/F= 14.36544 %FUEL= 6.508114 R, EQ. RATIO= 1.199696 PHI, EQ. RATIO= 1.200000				
THERMODYNAMIC PROPERTIES				
P, ATM		0.9869	4.9346	9.869
T, K		2136.49	2141.70	2142.95
RHO, G/CC		1.4927-4	7.4481-4	1.4889-3
H, CAL/G		-72.821	-72.821	-72.821
U, CAL/G		-232.94	-233.27	-233.35
G, CAL/G		-5224.14	-4978.43	-4870.03
S, CAL/(G) (K)		2.4111	2.2905	2.2386
M, (1/n)		26.515	26.526	26.529

The video feed shows a man in a white shirt and glasses, looking at the screen.

Let us just look at the Knox value at rich conditions the temperatures are lower as expected, let me not spend too much time on that.

(Refer Slide Time: 18:00)



SON VEL,M/SEC	911.6	915.4	916.4
MOLE FRACTIONS			
*Ar	0.00801	0.00802	0.00802
*CO	0.04517	0.04515	0.04515
*CO2	0.06267	0.06273	0.06275
*H	0.00064	0.00029	0.00021
*H2	0.02672	0.02666	0.02665
H2O	0.18778	0.18826	0.18838
*NO	0.00012	0.00005	0.00004
*N2	0.66822	0.66852	0.66859
*O	0.00001	0.00000	0.00000
*OH	0.00063	0.00030	0.00021
*O2	0.00003	0.00001	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

The NO is much much less than what it was at point h ok. So, there is no oxygen available, see the reactions are slow I mean even when you allow it to equilibrate there is not much oxygen that is available for NO to form because the conditions are already fuel rich I think that is probably the only take away from this calculation.

What, well there is there are variety of things that you can do we can do a rocket calculation and get the c star values, the molecular weight and you can even simulate quasi one-dimensional isentropic flow through a nozzle to you know estimate for a given area ratio you can estimate various things, assuming frozen equilibrium and frozen conditions or equilibrium conditions which I will mention we will discuss briefly tomorrow.

But what I would like to go from I can do many more examples, but probably it is going to be a little bit monotonous, but what I would suggest is that if you can give me some cases which

you want to be analyst, we can look at that. For example, some fuel oxidizer combinations from liquid rockets or solid rockets there are some combinations that you want to look at or have some specific questions we can discuss that.

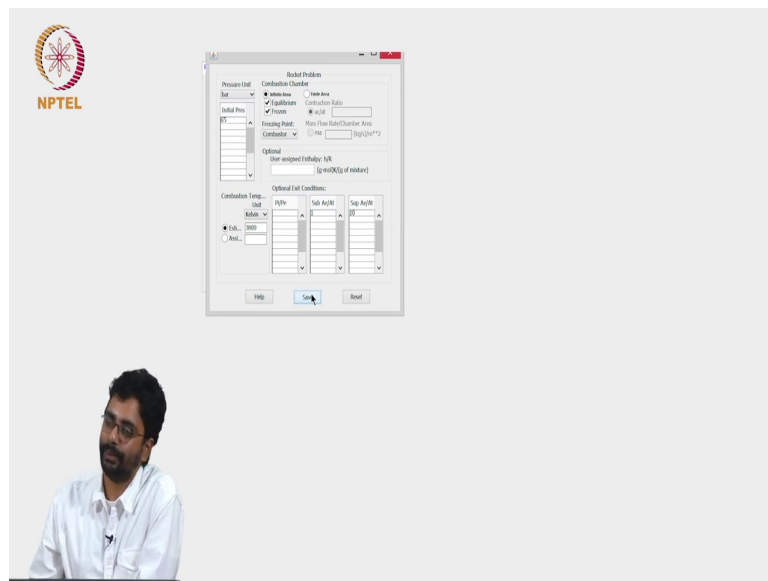
Student: (Refer Time: 19:15).

You want to do a rocket calc ok, why not?

Student: Tomorrow, we have do.

No, let us do, it is.

(Refer Slide Time: 19:29)



Student: Evaporation is around 65 bar.

Just.

Student: (Refer Time: 19:41).

Student: (Refer Time: 19:42).

Please correct me if I am putting the numbers in the wrong place.

Student: (Refer Time: 19:53) so we put one more it.

Yeah.

Student: (Refer Time: 19:56).

So, I should delete this right.

Student: Or we can put one only 0.

All right, ok, fine. Let us see what it means and.

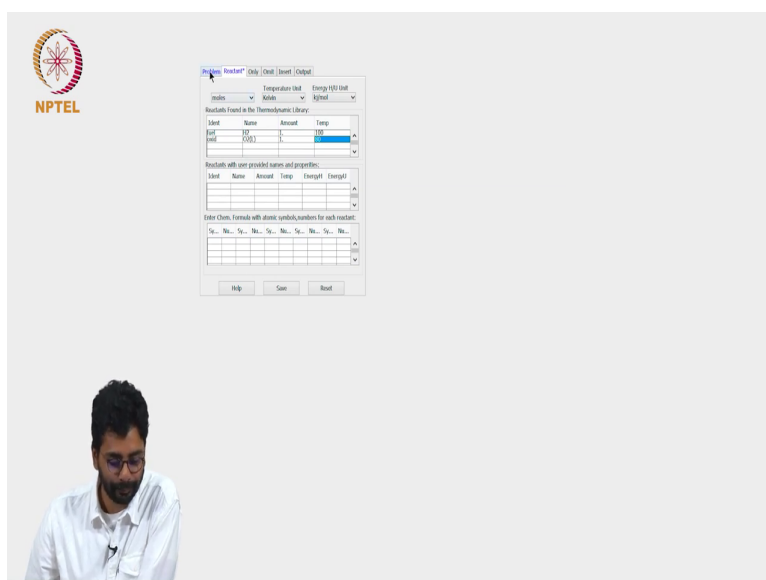
Student: One more thing was there estimated temperature that I (Refer Time: 20:16).

See that is only in initial guess that the code starts with.

Student: It starts hydrating.

It starts hydrating from that number you can giving closer number will make the iteration process faster that is it, there is no significant advantage beyond that.

(Refer Slide Time: 20:33)



Student: So, will I have liquid hydrogen (Refer Time: 20:36).

What is it one.

Student: (Refer Time: 20:45)

100 Kelvin's?

Student: (Refer Time: 20:47).

No, liquid hydrogen.

Student: Liquid hydrogen (Refer Time: 20:54).

No, we are interested in the thrust chamber or what happens later in the thrust chamber.

Student: At the ending of and (Refer Time: 21:03).

Student: At the ending of nozzle (Refer Time: 21:04).

No, the reactant condition at the inlet to the rocket thrust chamber would be gaseous hydrogen.

Student: (Refer Time: 21:17).

Yeah.

Student: The liquid temperature to that.

So, instead.

Student: (Refer Time: 21:22).

Instead you want to.

Student: Yes, yes.

Simulate the real condition.

Student: (Refer Time: 21:25).

The at the entry to the thrust chamber it will be in gaseous form the temperature that is less than a 100 Kelvin's.

Student: It is ok, but (Refer Time: 21:32).

Student: (Refer Time: 21:34) inlet to the thrust chamber.

Inlet to the thrust chamber is after the cooling.

Student: (Refer Time: 21:41).

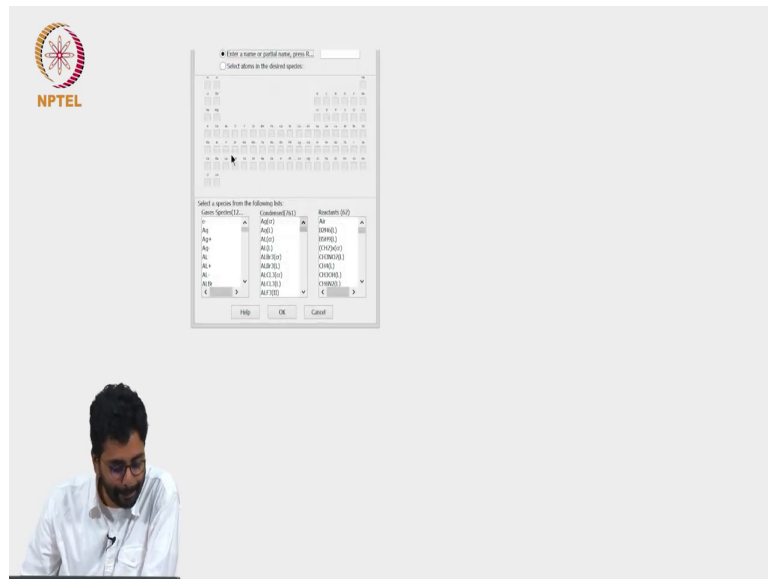
That is the point I am trying to make.

Student: Yes (Refer Time: 21:43).

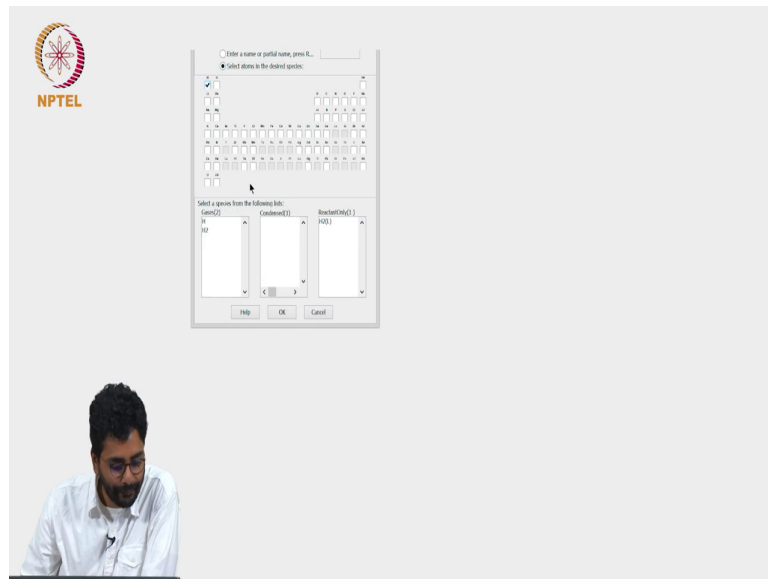
It goes the fuel cooling region rate of cooling happens and then it enters the thrust chamber. So, shall I make it gaseous hydrogen at 100 Kelvin's is the point that I am making.

Student: (Refer Time: 21:53).

(Refer Slide Time: 21:53)



(Refer Slide Time: 21:55)



And liquid oxygen, happen to remember the temperature sorry.

Student: 90 or 80 Kelvin's.

80 Kelvin's.

Student: 80 or 90.

Student: (Refer Time: 22:15) 80 Kelvin's.

80 Kelvin's is fine ok, and mixture ratio.

Student: (Refer Time: 22:19) 5 point 5.7 or something 5.7.

Student: 2 3.

Student: 81 to 4.8, 5 point.

Student: 5 point.

Student: 5.6.

And right let me see oxidizer to fuel weight ratio will be same as mixture ratio I guess give me some numbers.

Student: 5.7, 5.7.

This is the optimal this is the nominal.

Student: This is the operating minimum work.

You want something less and something more let us say 4.5 and.

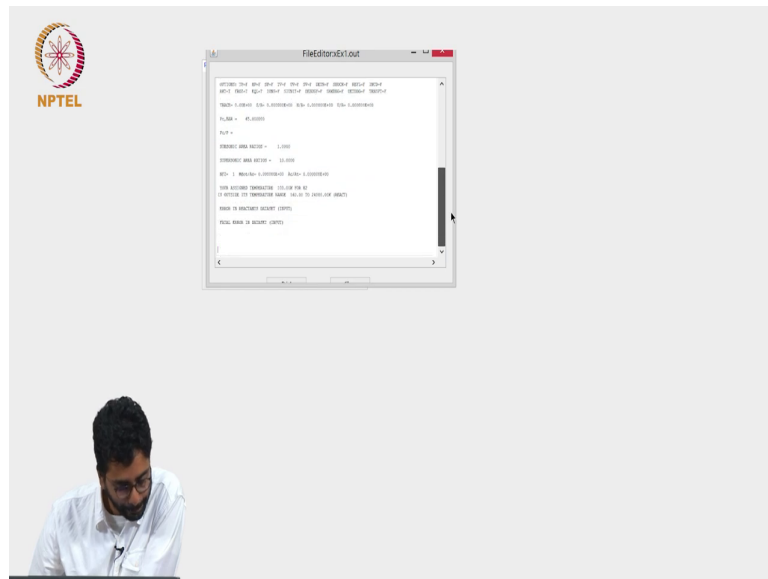
Student: (Refer Time: 22:48).

7, 6 point.

Student: 6.2.

6.2 ok. Let me see if it runs. It is unhappy with the data sets.

(Refer Slide Time: 22:57)

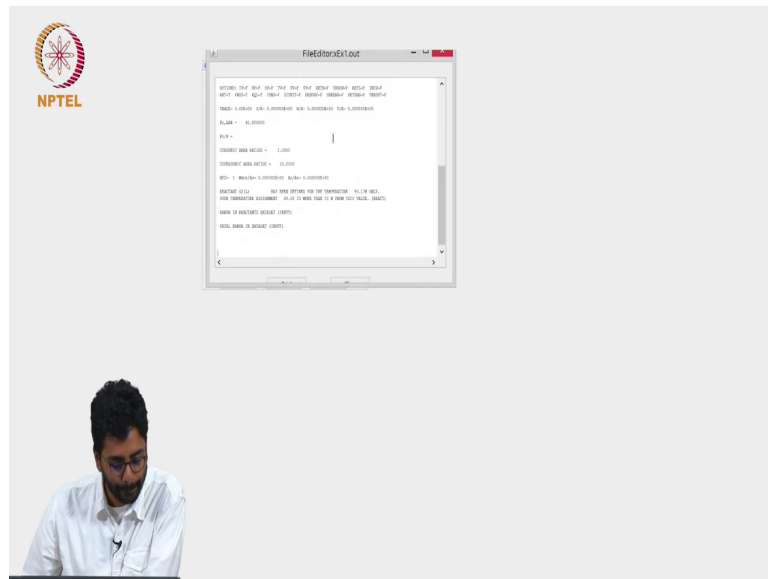


Student: (Refer Time: 23:06).

For logs for 1 h to the temperature range is a little limited I will give a little higher temperature.

Student: We will give 168, 61, 61, and we will give 161.

(Refer Slide Time: 23:28)



All right. Let us see is 80 is also.

Student: May be that gives 90.

Student: 90.

90.17.

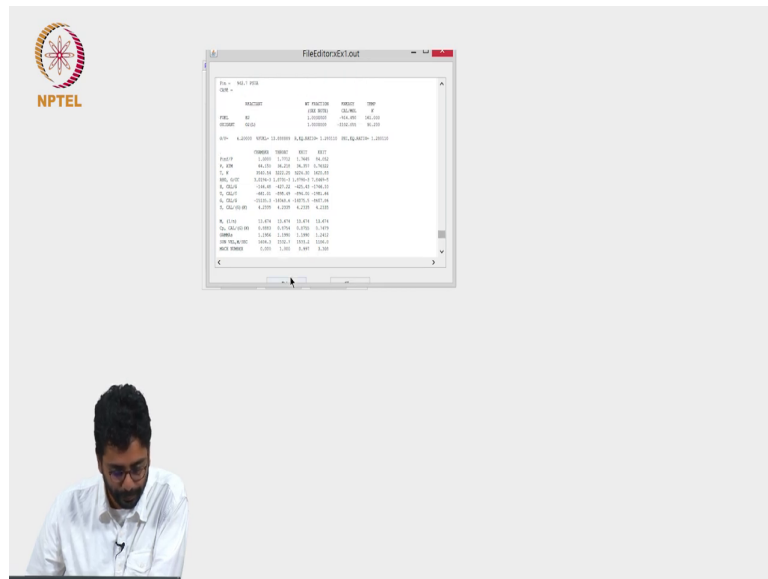
Student: 98, 90 90.

Yeah, ok.

(Refer Slide Time: 23:43)

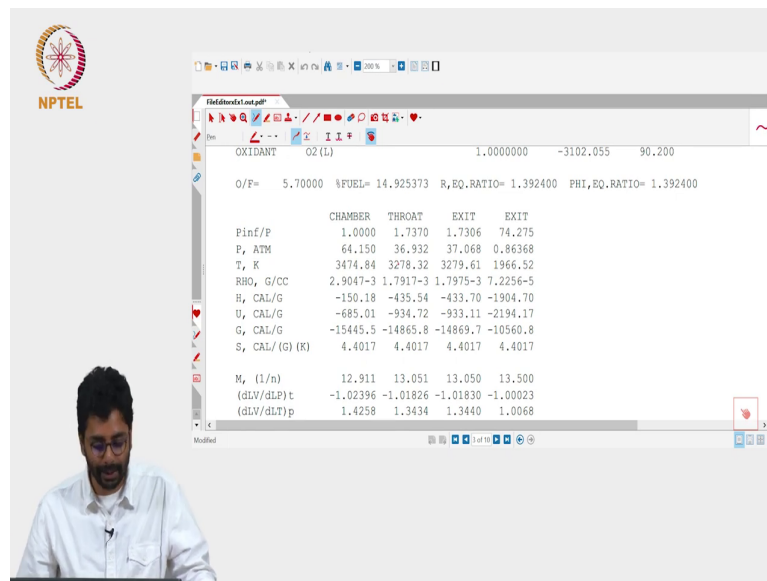
[illegible]

(Refer Slide Time: 23:49)



You want me to print it or you want to look at or add some more conditions, what do you want to look at?

(Refer Slide Time: 24:17)

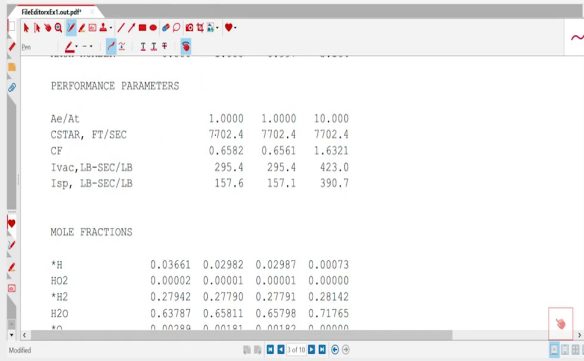


Student: Temperature whatever thrust chamber that is we are getting and also the composition species.

Student: (Refer Time: 24:15).

All right. This is for 5.7 that the number is visible for you actually I should not be looking in the other direction. Starts from 64 I am guessing that I have given the A by 80 correctly. So, it starts at 64 at throw it at 36. Well this is for the (Refer Time: 24:42) 80fl, there is no expansion. I think we should look at this case that is the exit temperature exit pressure is 0.86, ideal, this is the optimal expansion case I am guessing. So, the temperature is 3475 Kelvin's.

(Refer Slide Time: 25:05)



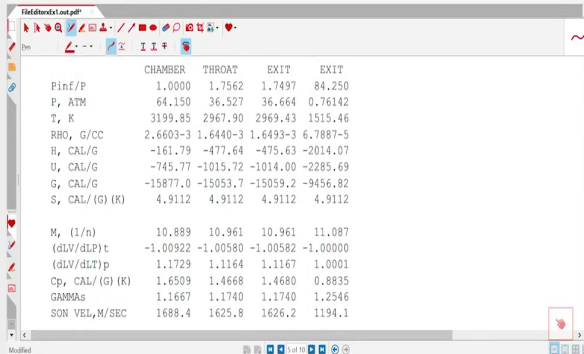
The screenshot shows a software window titled 'firedhorex1.out.pdf' with a toolbar and a scrollable area. The scrollable area contains two sections: 'PERFORMANCE PARAMETERS' and 'MOLE FRACTIONS'. The 'PERFORMANCE PARAMETERS' section has a table with 5 rows and 4 columns. The 'MOLE FRACTIONS' section has a table with 5 rows and 4 columns. A man is visible in the bottom left corner of the frame.

PERFORMANCE PARAMETERS			
Ae/At	1.0000	1.0000	10.000
CSTAR, FT/SEC	7702.4	7702.4	7702.4
CF	0.6582	0.6561	1.6321
Ivac, LB-SEC/LB	295.4	295.4	423.0
Isp, LB-SEC/LB	157.6	157.1	390.7

MOLE FRACTIONS			
*H	0.03661	0.02982	0.02987
H2	0.00002	0.00001	0.00001
*H2	0.27942	0.27790	0.27791
H2O	0.63787	0.65811	0.65798
H2O	0.00259	0.00181	0.00182

C star is it is in I did not change the units it is in feets per second, 7700. So, 5.7, the c star is 7700 which condition is this. This is also 5.7 ok, ok. I think one is frozen; the other is equilibrium probably.

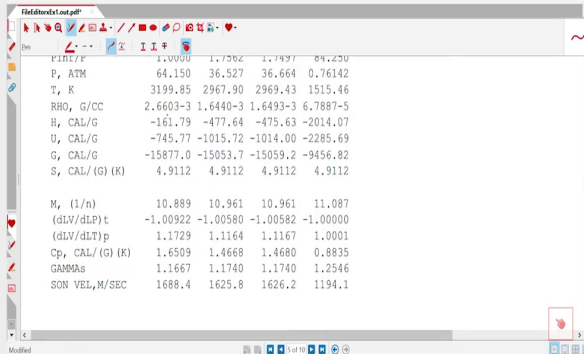
(Refer Slide Time: 25:36)



	CHAMBER	THROAT	EXIT	EXIT
Pinf/P	1.0000	1.7562	1.7497	84.250
P, ATM	64.150	36.527	36.664	0.76142
T, K	3199.85	2967.90	2969.43	1515.46
RHO, G/CC	2.6603E-3	1.6440E-3	1.6493E-3	6.7887E-5
H, CAL/G	-161.79	-477.64	-475.63	-2014.07
U, CAL/G	-745.77	-1015.72	-1014.00	-2285.69
G, CAL/G	-15877.0	-15053.7	-15059.2	-9456.82
S, CAL/(G) (K)	4.9112	4.9112	4.9112	4.9112
M, (l/n)	10.889	10.961	10.961	11.087
(dLV/dLP)t	-1.00922	-1.00580	-1.00582	-1.00000
(dLV/dLT)p	1.1729	1.1164	1.1167	1.0001
Cp, CAL/(G) (K)	1.6509	1.4668	1.4680	0.8835
GAMMA	1.1667	1.1740	1.1740	1.2546
SON VEL, M/SEC	1688.4	1625.8	1626.2	1194.1

This is 4.5, your temperatures have gone down it is 3200, the c star would have also gone down.

(Refer Slide Time: 25:44)

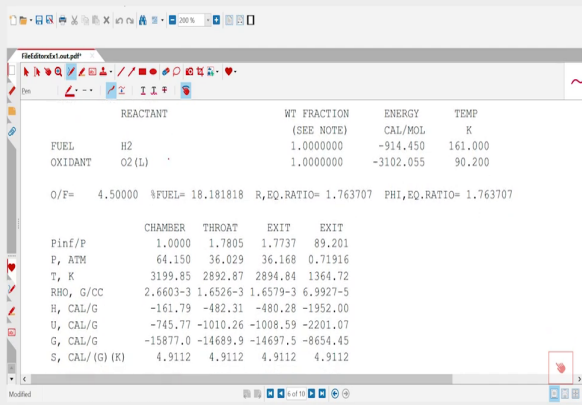


The screenshot shows a text editor window titled 'filed100.txt notepad'. It contains a table of thermodynamic properties for water at 100°C. The properties are listed in two columns, with the first column being the property name and the subsequent columns being numerical values. The properties include P, ATM; T, K; RHO, G/CC; H, CAL/G; U, CAL/G; G, CAL/G; S, CAL/(G) (K); M, (l/n); (dlV/dLP)t; (dlV/dLT)p; Cp, CAL/(G) (K); GAMMA_S; and SON VEL, M/SEC.

Property	Value 1	Value 2	Value 3	Value 4
P, ATM	1.0000	1.7362	1.7497	89.250
T, K	64.150	36.527	36.664	0.76142
RHO, G/CC	3199.85	2967.90	2969.43	1515.46
H, CAL/G	2.6603-3	1.6440-3	1.6493-3	6.7887-5
U, CAL/G	-161.79	-477.64	-475.63	-2014.07
G, CAL/G	-745.77	-1015.72	-1014.00	-2285.69
S, CAL/(G) (K)	-15877.0	-15053.7	-15059.2	-9456.82
M, (l/n)	4.9112	4.9112	4.9112	4.9112
(dlV/dLP)t	10.889	10.961	10.961	11.087
(dlV/dLT)p	-1.00922	-1.00580	-1.00582	-1.00000
Cp, CAL/(G) (K)	1.1729	1.1164	1.1167	1.0001
GAMMA_S	1.6509	1.4668	1.4680	0.8835
SON VEL, M/SEC	1.1667	1.1740	1.1740	1.2546

Of course that is the c star comes downstream. Now, let me ask a different question you have let us say you have got a temperature from here you have got a c star from here.

(Refer Slide Time: 25:56)

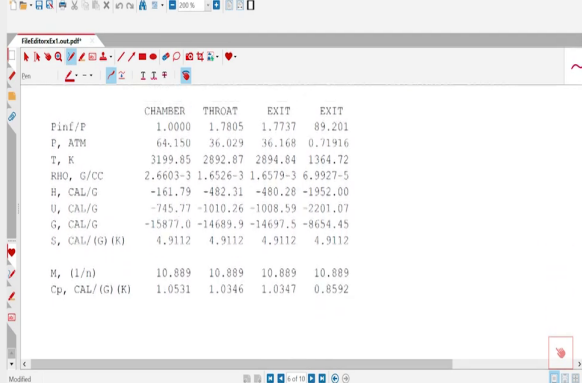


The screenshot displays a software window titled "firedirect.txt.pdf" showing the results of a combustion calculation. The window is divided into several sections. The top section lists the reactants: FUEL (H2) and OXIDANT (O2 (L)). Below this, the O/F ratio is given as 4.50000, and the %FUEL is 18.1818. The R, EQ, RATIO is 1.763707, and the PHI, EQ, RATIO is 1.763707. The bottom section shows a table of properties for the CHAMBER, THROAT, and EXIT (two columns). The properties listed are Pinf/P, P, ATM, T, K, RHO, G/CC, H, CAL/G, U, CAL/G, G, CAL/G, and S, CAL/(G) (K).

	CHAMBER	THROAT	EXIT	EXIT
Pinf/P	1.0000	1.7805	1.7737	89.201
P, ATM	64.150	36.029	36.168	0.71916
T, K	3199.85	2892.87	2894.84	1364.72
RHO, G/CC	2.6603-3	1.6526-3	1.6579-3	6.9927-5
H, CAL/G	-161.79	-482.31	-480.28	-1952.00
U, CAL/G	-745.77	-1010.26	-1008.59	-2201.07
G, CAL/G	-15877.0	-14689.9	-14697.5	-8654.45
S, CAL/(G) (K)	4.9112	4.9112	4.9112	4.9112

Let us say you wanted to further calculations how do you decide that this number is a good approximation to work with as in this is an equilibrium calculation, and you want to use it for further calculation. The question that I would like to post and discuss is how do we decide that the reactants would have reacted and reached a state that is sufficiently close to equilibrium before the expansion through the nozzle starts that is an important question to ask and discuss.

(Refer Slide Time: 26:25)

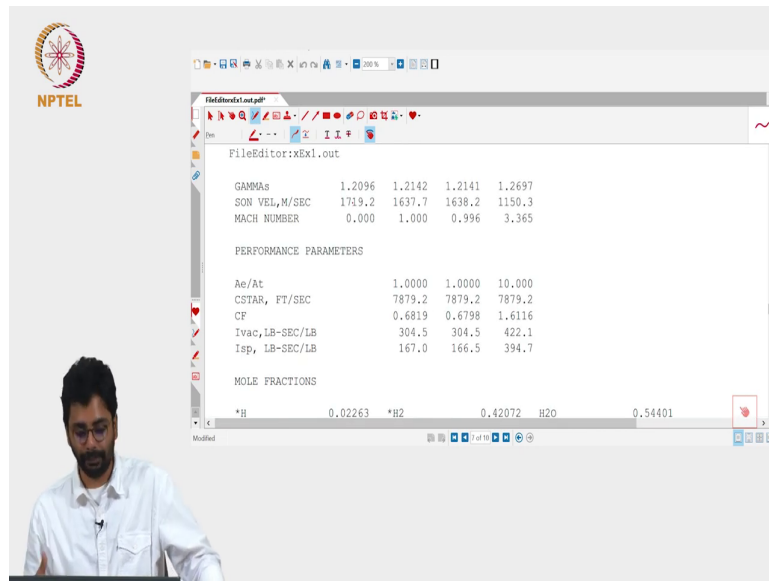


	CHAMBER	THROAT	EXIT	EXIT
P_{in}/P	1.0000	1.7805	1.7737	89.201
P , ATM	64.150	36.029	36.168	0.71916
T , K	3199.85	2892.87	2894.84	1364.72
RHO , G/CC	2.6603×10^{-3}	1.6526×10^{-3}	1.6579×10^{-3}	6.9927×10^{-3}
H , CAL/G	-161.79	-482.31	-480.28	-1952.00
U , CAL/G	-745.77	-1010.26	-1008.59	-2201.07
G , CAL/G	-15877.0	-14689.9	-14697.5	-8654.45
S , CAL/(G) (K)	4.9112	4.9112	4.9112	4.9112
M , (1/n)	10.889	10.889	10.889	10.889
C_p , CAL/(G) (K)	1.0531	1.0346	1.0347	0.8592

How much time do you think it requires for hydrogen oxygen system to reach equilibrium and how much time is available in an actual rocket engine?

Student: So, may be have a maybe 4 times (Refer Time: 26:39) 4 to 6 times.

(Refer Slide Time: 26:43)



The screenshot shows a video lecture interface. In the bottom left corner, a man with glasses and a white shirt is visible. The main part of the screen displays a text editor window titled 'FileEditor:xEk1.out'. The text in the window is as follows:

```
FileEditor:xEk1.out

GAMMAS      1.2096  1.2142  1.2141  1.2697
SON VEL,M/SEC 1749.2  1637.7  1638.2  1150.3
MACH NUMBER   0.000   1.000   0.996   3.365

PERFORMANCE PARAMETERS

Ae/At        1.0000  1.0000  10.000
CSTAR, FT/SEC 7879.2  7879.2  7879.2
CF           0.6819  0.6798  1.6116
Ivac, LB-SEC/LB 304.5  304.5  422.1
Isp, LB-SEC/LB 167.0  166.5  394.7

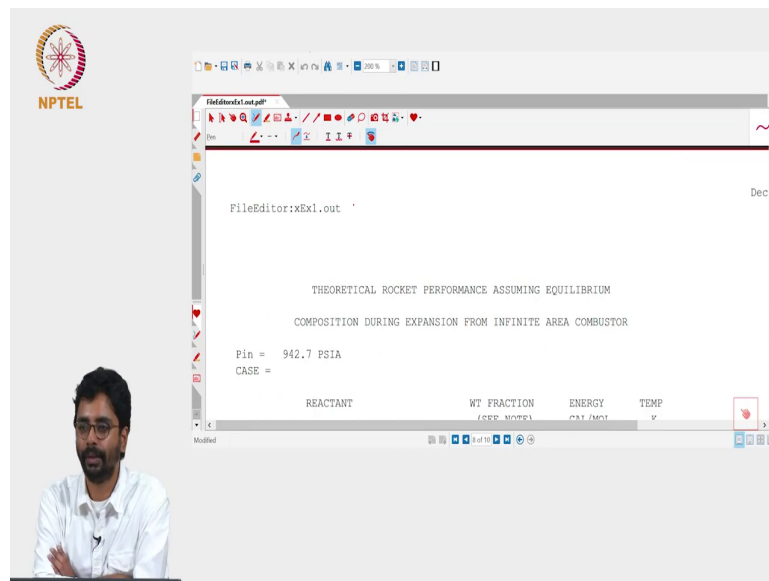
MOLE FRACTIONS

*H           0.02263  *H2           0.42072  H2O           0.54401
```

And how do you get an estimate for the time?

Student: For the reaction time?

(Refer Slide Time: 26:48)



What is the typical reaction time for hydrogen?

Student: Oxygen time.

Oxygen, yes, no, unless we know that we cannot decide whether there is sufficient time. Of course, the time that is available for the reactants inside the combustion chamber can be calculated from the in approximate velocity which is the reactance move.

Student: They enter inside.

Enter inside and move through the combustion chamber, and length divided by that velocity will give us a good estimate of the time that the reactants.

Student: Spend inside the combustion chamber.

Spend inside the combustion chamber. And the way the injectors are arranged it will also be a reasonable approximate assumption to make that reactants are sufficiently mixed at a certain distance downstream which we can subtract from the length of the combustion chamber. So, from that starting from that point onwards, where the reaction between hydrogen and oxygen starts where it is injected in a coaxial fashion and it reaches the nozzle how can may be sure that it has reached equilibrium. So, is my question clear?

Student: Yeah.

For and this is routinely used for calculation and that is the reason why I want to discuss this yeah. Let us start by getting a simple estimate for the time that is available in a rocket engine.

Student: Hope we have a (Refer Time: 28:08).

Ok.

Student: And the mixing time mixing them (Refer Time: 28:14) of may combustion is getting it is may be some 90 percent of l let us start.

90 percent of l, what is?

Student: (Refer Time: 28:22).

Let us take; let us take the specific engine.

Student: Yes.

What is the length?

Student: If we take our one of the engine there is some 500 to 600 mm.

Let us say 500 mm ok.

Student: Then the mixing range will be approximately from 40 to 60y second 40 to 60.

Fine, may be take it as a 500 millimeters.

Student: Yes.

The number that is easy to work with.

Student: 500 mm.

Half a meter yes.

Student: After that we will have a mixing zone there the sorry automation mixing zone.

Correct.

Student: Then they are coming to the reaction zone.

Yeah.

Student: There we will consider almost like whatever we are discussing like where very infinite reaction rate.

Very fast reactions have happened.

Student: Very fast reactions happened.

So, the.

Student: Then coming to the equilibrium establishment from that we will have really 1.5 times normal for attaining the equilibrium.

What is 1.5 times the margin? I am trying to estimate a time.

Student: Suppose if we.

Yeah.

Student: Has the If I entire combustion reaction is taking into some 250 mm.

Right.

Student: That 250 mm enter (Refer Time: 29:17).

So, the length available for the reaction you would say is 250 millimeters.

Student: Yes.

And what do you think is a good estimate for the velocity in that region, the actual velocity in that region.

Student: Axial velocity in that is 0.

Now, you will take 0.

Student: Yes.

That is fine.

Student: That is.

Then because you want to assume that there is large time available for the reactions time.

Student: Yes.

In happening in reality how much would be the velocity?

Student: It depends on the temperature that we are really getting it.

Yeah.

Student: And from that using kinetic energy we will calculate what is the molecular, pre molecular velocity? You do not need the pre molecular velocity.

Student: (Refer Time: 29:51)

What I am what we need is simply the mass flux.

Student: Yes.

At a given section divided by the cross section area.

Student: cross section area divided by the density.

Divided by the density. So, that you would say is 100 meters per second, 200 meters per second or how much is it hm.

Student: (Refer Time: 30:08).

Is 100 meters per second a good value?

Student: (Refer Time: 30:13).

Student: Ha.

Fine. So, we have.

Student: T to 100 meters yes.

So, 0.25 meters is the distance that is available and a 100 meters per second is the velocity.

Student: Velocity.

So, 0.25 divided by 100 is the time that is available.

Student: Yes.

And that is.

Student: Sir point 2.5.

2.5 milliseconds correct. So, it is 2.5 milliseconds sufficient for a mixture of hydrogen oxygen.

Student: To reach equilibrium.

To reach equilibrium, yes, why?

Student: Because (Refer Time: 30:40) for these conditions is varying.

Ok.

Student: Your pressurizing the system chamber at 60 bar or something 60 bar.

60 bar ok.

Student: And for the for the log systems a at the 1 atmospheric pressure 1 itself lamina flame is speed is 3.

Ok.

Student: If you go to up to that high pressures it will reactivity goes by square of pressure.

Ok.

Student: So, that laminar flame speed is under root of lamina reactivity is under lamina flame speed is under root of reactivity that is means lamina flame speed go linearly with pressure. So, it will increase.

Student: Yes.

Well, that no that analysis will show if you assume a the reactions to be effectively by molecular that the.

Student: Correct.

Flame speed is incisive to pressure ok.

Student: I think we have we have not so (Refer Time: 31:28).

So, that is one thing.

Student: But.

Even then.

Student: It will be increasing.

Even then is the approximation reasonable.

Student: Yes.

So, if you what number for reaction time would you get is the followed the same procedure that I described in the morning, I suggest that you please think about that see we have got one estimate for times which is 2.5 milliseconds, the other estimate that we need to get is a timescale for the reactions to go to completion which as he rightly pointed out can be obtained from an approximate value for the flame speeds ok.

Student: Flame speed.

Please plug in some numbers and see if this approximation that we that you regularly use to calculate equilibrium composition, and use it for various things you know expansion through the nozzle and various heat transfer calculations and so on. Is it a reasonably good

approximation or not, it is something I would like you to go back and check and we can discuss it next class or tomorrow ok. That is one good example that we have looked at.

Student: Sir, we have one (Refer Time: 32:35)

Just before that I just want to make sure, but you are looking for anything something else when you post this question?

Student: Right.

Is that it ok.

Student: The reason being we have been updated one of the (Refer Time: 32:48).

Student: 58 bar (Refer Time: 32:51) so 64 bar.

Ok.

Student: Just for increasing the thrust and I have reached.

Student: Just remain the same, but thrust can be increased.

Student: So, in that context when we are running this CEA in one of the processing that we are going discussing for the quite longer the temperature also and quite got increasing nearly you know (Refer Time: 33:13).

As I mentioned that the benefit that you will get because of you know lesser decomposition at higher pressures will saturate beyond a certain value of pressure.

Student: but the dissociation reaction that we have not actually we have not considered them, but after some maturity of understanding both the dissociation reactions we nearly added to the right number may be from, 480 Kelvin.

I also would not expect that the benefit because of increase in pressure in terms of temperature would be.

Student: (Refer Time: 33:46).

Significant because you are going from already a pressure that is

Student: Yes.

Significant I mean that is sufficiently high, it was slightly higher pressure.

Student: Everything is for this increasing chamber pressure, the same mixture ratio, obviously mixture ratio only control the complete process.

Yes.

Student: While since it is not shifting much you got at the same number onwards.

Yeah.

Some learning that you had ok. I just stop before we move on I just wanted to since the topic of c star came up. I quickly sort of went through that in the morning I just want to ok.

(Refer Slide Time: 34:33)



Combustion for propulsion: Fundamentals

S Varunkumar and H S Mukunda

NPTEL course-cum-workshop, 19-22, December, 2019



So, the point when the presentation loads the point that I want to make is that a for hydrogen oxygen system, the flame temperature will like for any other system will peak around stoichiometry.

(Refer Slide Time: 34:52)



What combustion fundamentals will real systems need?



(Refer Slide Time: 34:53)



Equilibrium



But the c star value which is a parameter that is a measure of performance in an actual rocket will peak at which conditions ok.

(Refer Slide Time: 34:58)



Relative fluctuation and continuum assumption

For average properties to be meaningful, the average number of molecules in a chosen volume should be large enough for the fluctuations created by the random molecular motion to be negligible.

This is quantified using the so called "relative fluctuation" - this is the ratio of the standard deviation of the number of molecules in a given volume to the average number of molecules in that volume.

For ideal gases, the relative fluctuation is inversely proportional to the square root of the average number of molecules.

$$\text{relative fluctuation} = \frac{\Delta N}{N} \sim \frac{1}{\sqrt{N}} = \sqrt{\frac{RT}{pV N_A}}$$

$p = 1 \text{ atm and } 1000 \text{ K}$

$d \text{ (}\mu\text{m)}$	relative fluctuation (%)
0.01	51
0.1	1.6
1	0.051
10	0.0016
100	5.1×10^{-5} (51 ppm)
1000	1.6×10^{-6} (1.6 ppm)

Because the c star is also dependent or c star is proportional to be sound speed ok.

(Refer Slide Time: 35:03)



$$t_r = \frac{\text{mass per volume of the flame (kg/m}^3\text{)}}{\text{speed of chemical reaction (kg/m}^2\text{-s)}} = \frac{\rho}{\dot{\omega}}, \quad \dot{\omega} \sim \frac{c_a}{k} (\rho_u S_u)^2$$

- we will see later how this comes about. Plugging

this into the expression for δ , we get,

$$\delta = \frac{\alpha}{S_u}, \quad S_u \text{ is the flame speed, a measure of the reactivity of a fuel-oxidizer mixture, which is simpler to measure compared to } \dot{\omega}$$

Fuel - oxidizer	S_u (m / s)	δ (μ m)
Hydrogen - Air	3	33
Hydrogen - Oxygen	20	5
Methane - Air	0.4	250
Methane - Oxygen	4	25



So, smaller the molecular weight, larger is the sound speed.

(Refer Slide Time: 35:07)



- The thickness over which the temperature change is significant is much larger than what is required for the continuum assumption to be valid. Therefore, in a volume about the thickness of the flame, we can ask questions of the following sort -

(1) What is the temperature of the flame?

(2) What is the chemical composition of the products of combustion?

- These are the meaningful questions for which Thermodynamics can provide answers.
- Its clear that the length scales are such that the laws of thermodynamics can be applied.
- But what about time scales? Convince yourselves that the time scales involved also satisfy the conditions to apply the laws of thermodynamics.



(Refer Slide Time: 35:08)



Quick overview of laws of thermodynamics

First law : $\delta q - \delta w = dU \Rightarrow \delta q = dU + pdV = dH - vdP$

Second law : $dS_{\text{system}} + dS_{\text{surroundings}} \geq 0$

$dS_{\text{surroundings}} = \frac{-\delta q}{T_{\text{surroundings}}} = \frac{-(dU + pdV)}{T_{\text{surroundings}}} = \frac{-(dH + Vdp)}{T_{\text{surroundings}}}$; substituting this in the expression for second law,

$dS_{\text{system}} - \frac{dU + pdV}{T_{\text{surroundings}}} \geq 0 \Rightarrow dU + pdV - T_{\text{surroundings}} dS_{\text{system}} \geq 0 \rightarrow \text{minimum}$

Helmholtz free energy

(or)

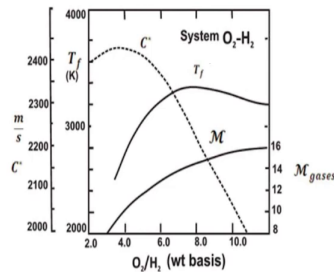
$dS_{\text{system}} - \frac{dH - Vdp}{T_{\text{surroundings}}} \geq 0 \Rightarrow dH - Vdp - T_{\text{surroundings}} dS_{\text{system}} \geq 0 \rightarrow \text{minimum}$

Gibbs free energy



And c star values will be much higher when you have a large amounts of hydrogen because the molecule weights are significantly lesser than oxygen.

(Refer Slide Time: 35:18)



So, So, the as you can see from this the flame temperature peaks at a mixture ratio for around 8 which is the stoichiometric a mixture ratio for oxygen hydrogen system. But this c star which is a dotted line reaches a maximum at a mixture ratio between I would say it is 4 and 5 ok. And in that is a kind of number that is also used in actual systems where the c star is maximum not necessarily where temperature is maximum.

Student: In this c star something that pc 80 by m dot.

PC 80 m dot and it is also proportional to square root of.

Student: (Refer Time: 35:56).

Square root of the temperature divided by the molecular weight, divided by the square root of the molecular weight. So, it will peak. So, as you can see T_f is maximum at 8, but molecule weight is significantly lower between 4 and 5 compared to stoichiometric values, and therefore, square root of T_f by square root of M will reach a maximum at which conditions when there is lot more hydrogen ok. Of course, you cannot go further in to the left of it, but at some point between 4 and 6, it reaches the maximum ok.